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## **Demonstration Applications of ARAMS for Aquatic and Terrestrial Ecological Risk Assessment**

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**ABSTRACT:** The Adaptive Risk Assessment Modeling System (ARAMS) has been developed for the Army to provide the capability to conduct risk assessments associated with exposure to constituents of potential concern. ARAMS provides a reliable and repeatable methodology for conducting collaborative and comparative risk assessments, thus providing a savings in time and cost for conducting such assessments and potentially leading to significant remediation cost savings by providing more accurate risk-based cleanup targets. The objectives of this study were to describe and demonstrate the application of ARAMS for ecological risk characterization at two field sites, an aquatic site and a terrestrial site. Other purposes of the study were to identify errors and data/development gaps, and to validate methods and solutions of ARAMS and its components for ecological risk assessment. ERDC researchers, through literature searches and communications with personnel at the Corps of Engineers Center of Expertise for Hazardous, Toxic, and Radiological Waste and Corps districts, identified potential demonstration sites. The candidate sites, which are or were owned or operated by the U.S. Army, Navy, or Air Force, were either components of Superfund projects or were Formerly Used Department of Defense Sites. Langley Air Force Base (LAFB) and Pueblo Chemical Depot (PCD) were selected among the identified sites to demonstrate the capabilities of ARAMS. The reported ecological risk assessments for LAFB and PCD sites were used to obtain data for conducting these demonstrations. At LAFB, risks were evaluated for benthic invertebrates, a fish (Atlantic croaker), a piscivorous bird (belted kingfisher), and a carnivorous mammal (mink). The selected chemicals of concern at LAFB were polychlorinated biphenyls, benzo(a)pyrene, and arsenic. At PCD, risks to a primary consumer/omnivore (deer mouse), an upper-trophic level mammalian predator (swift fox), and two upper trophic level avian predators (ferruginous hawk and western meadowlark) were evaluated. The chemicals of concern at PCD were 2,4,6-trinitrotoluene, 2,4-dinitrotoluene, 2,6-dinitrotoluene, cyclotetramethylene-tetrannitramine, and 1,3,5-trinitrobenzene. These applications illustrate a number of ARAMS features, including media fate and transport, access to aquatic and terrestrial databases to extract wildlife toxicity benchmarks, and calculations of exposure doses and hazards quotients.

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# **Conversion Factors, Non-SI to SI Units of Measurement**

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Non-SI units of measurement used in this report can be converted to SI units as follows:

Multiply	By	To Obtain
acres	4,046.873	square meters
feet	0.3048	meters
miles (U.S. statute)	1.609347	kilometers

# Preface

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This report describes the application and demonstration of the Adaptive Risk Assessment Modeling System (ARAMS) to selected sites for aquatic and terrestrial ecological risk assessment. Drs. Mansour Zakikhani and Dennis L. Brandon of the Environmental Processes and Engineering Division (EPED) of the Environmental Laboratory (EL), U.S. Army Engineer Research and Development Center (ERDC), Vicksburg, MS, conducted these applications and prepared this report. Dr. Mark S. Dortch and Mr. Jeffrey A. Gerald, Water Quality and Contaminant Modeling Branch (WQCMB), EPED, contributed to this report.

This work was conducted as part of the Hazard/Risk Focus area of the U.S. Army Environmental Quality Technology Research and Development Program, Dr. John Cullinane, program manager. This work was conducted under the general supervision of Dr. Barry Bunch, Chief, WQCMB, and Dr. Richard E. Price, Chief, EPED. Dr. Beth Fleming was Acting Director of EL.

COL James R. Rowan, EN, was Commander and Executive Director of ERDC, and Dr. James R. Houston was Director.

# 1 Introduction

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## Background

The U.S. Department of Defense and the Army conduct risk assessments to determine safe exposure levels and cleanup target levels for military relevant compounds (MRCs)<sup>1</sup> and to evaluate remediation alternatives to provide the most cost-effective approach to reach target levels. An Adaptive Risk Assessment Modeling System (ARAMS) has been developed for the Army through the Environmental Quality Technology Research and Development Program to provide the capability to conduct risk assessments associated with exposure to constituents of potential concern (COPC). ARAMS provides a reliable and repeatable methodology for conducting collaborative and comparative risk assessments, thus providing a savings in time and cost for conducting such assessments and potentially leading to significant remediation cost savings by providing more accurate risk-based cleanup targets. ARAMS is based on the widely accepted risk paradigm that integrates exposure and effects assessments to characterize risk. The object-oriented conceptual site model (CSM) is the central assessment mechanism in ARAMS. The CSM is based on the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) developed by Battelle Memorial Institute of the Pacific Northwest National Laboratory (PNNL) of the U.S. Department of Energy (DOE). FRAMES was developed in cooperation with the U.S. Environmental Protection Agency (USEPA), DOE, the Nuclear Regulatory Commission, and the U.S. Army Engineer Research and Development Center (ERDC).

This document describes the application of ARAMS/FRAMES to an aquatic site and a terrestrial site for ecological risk assessment. These applications were conducted to demonstrate the utility of ARAMS for ecological risk assessment (ERA), as well as to expose development gaps for subsequent revision, and to validate ARAMS against actual ERAs. It is emphasized that these demonstrations are in no way intended to replace or complement the previously reported assessments; rather they were conducted for ARAMS evaluation purposes.

These applications illustrate a number of ARAMS features, including media fate and transport, access to aquatic and terrestrial databases to extract wildlife toxicity benchmarks, and calculations of exposure doses and hazards quotients. These applications utilized ARAMS version 1.2 with FRAMES version 1.5. The

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<sup>1</sup> Appendix A contains a list of abbreviations and acronyms.

ARAMS Web site for download and other information is  
<http://el.erdc.usace.army.mil/arams>.

ERDC researchers, through literature searches and communications with the Corps of Engineers Center of Expertise for Hazardous, Toxic, and Radiological Waste personnel and Corps district personnel, identified potential demonstration sites. The candidate sites, which are or were owned or operated by the U.S. Army, Navy, or Air Force, were either components of Superfund projects or were Formerly Used Department of Defense Sites (FUDS). Langley Air Force Base (LAFB) and Pueblo Chemical Depot (PCD) were selected among the identified sites to demonstrate the capabilities of ARAMS. The reported ERAs for LAFB and PCD sites were used to obtain data for conducting these demonstrations.

URS Corporation (2002b) provided data and reports on ecological evaluation of LAFB. The data include several sediment, surface water, and biota sampling events between 1990 and 1997. Historical data could be used to calculate future risks. In addition to the screening-level ecological risk assessment (SERA), ERA, and human health risk assessment (HHRA) evaluations also have been reported. URS Corporation (2002b) provided lists of the sediment, water, and animal tissue data utilized in the remedial investigation. The site for aquatic ecological demonstration is located near the Back River in Virginia. At LAFB, risks were evaluated for benthic invertebrates, a fish (Atlantic croaker), a piscivorous bird (belted kingfisher), and a carnivorous mammal (mink). The selected chemicals of concern at LAFB were polychlorinated biphenyls (PCBs), benzo(a)pyrene, and arsenic.

Earth Tech (2002) summarized the SERA conducted at PCD. The PCD has several contaminated units of solid waste management units (SWMUs). The site for this demonstration is the TNT Washout Facility and Discharge System (SWMU 17), which is located within a short-grass prairie community and adjacent to an open-water area. SWMU 17 was a good site to demonstrate the capabilities of ARAMS in the terrestrial environment. At PCD, risks to a primary consumer/omnivore (deer mouse), an upper trophic level mammalian predator (swift fox), and two upper trophic level avian predators (ferruginous hawk and western meadowlark) were evaluated. The chemicals of concern were 2,4,6-trinitrotoluene (TNT), 2,4-dinitrotoluene, 2,6-dinitrotoluene, cyclotetramethylene-tetranitramine (HMX), and 1,3,5-trinitrobenzene (TNB).

## Objectives

The objectives of this study were to describe and demonstrate the application of ARAMS for ecological risk characterization at two field sites, an aquatic site (LAFB) and a terrestrial site (PCD). Other purposes of the study were to identify errors and data/development gaps, and to validate methods and solutions of ARAMS and its components for ERA.

## **Scope of Study**

The study started with selection of two sites from a list of 21 sites that have reports on ERAs. The data from the selected sites were obtained and analyzed. Next, site data were extracted from the reference documents and used to set up the ARAMS applications. ARAMS was applied and evaluated. Any problems noted in the applications were reported for necessary corrections. The details of these applications and the findings are documented in this report.

Site selection is discussed in Chapter 2, model theory is presented in Chapter 3, and the aquatic and terrestrial applications are presented in Chapters 4 and 5, respectively. Chapter 6 presents a summary of results with conclusions and recommendations.

## **2 Site Selection Criteria**

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A total of 21 military and civilian sites were considered for application (Table 1). Because of time and budget constraints, only two sites from the list in Table 1 were used in this study. The general criteria that were used in site selection are outlined below.

- a. The contaminants of concern (COC) included MRCs.
- b. An ERA report with fairly extensive assessments exists.
- c. A thorough ecological CSM was developed.
- d. Multiple exposure pathways were considered.
- e. Site determinations, e.g., ecological hazard quotients (EHQ) had been made.
- f. Recent site data of relatively high quantity and quality exist. Lower priority was given to older data.
- g. Availability of sufficient information for application of fate and transport models.
- h. The original source of contamination was well defined.

Additionally, Army sites were given a higher priority because of the ARAMS sponsoring source.

Two sites from Table 1, LAFB and PCD, which both had completed ERAs, were selected for the demonstration.

### **Langley Air Force Base**

URS Corporation (2002b) provides an extensive LAFB database, which includes several sediment, surface water, and biota sampling events between 1990 and 1997. Historical data are available, which can be used to calculate future risks. The main reason for the selection of this site was that the ERAs were available. URS Corporation (2002b) lists the sediment, water, and animal tissue data utilized in the remedial investigation (RI). This demonstration focuses on a sub-reach of the Back River (Southwestern Branch). This sub-reach is approximately 3,000 m long and 100 m wide. The average water depth is 1.5 m. More information about the site is given in Chapter 4.

<b>Table 1</b> <b>List of Potential Demonstration Sites</b>				
ID	Site	Owner/POC	Contaminant/Medium	Risk Assessment Status
1	Granite Canyon	State of CA (FUDS)/ P. Broderick	PCBs/Aquatic/Terrestrial	Ongoing
2	Hamilton Army Airfield	Army (FUDS)/ J. McAlister	Metals, VOCs, SVOCs, PCBs, PAHs/Aquatic/Terrestrial	RI/FS, ERA Completed
3	Fort Richardson (SS), AK	Army/R. Nenahlo	TNT, DNT, HMX/Soil, Water/Aquatic	RI/FS, ERA Completed
4	US Moorings (SS), OR	Army/S. Lemlich	Metals, Pesticides, SVOCs, DDT, TBT/ Aquatic/Terrestrial	Preliminary Data
5	Peoria Lake, IL	Civil	No Contaminant Data/ Plants/Aquatic	Turbidity, ERA Completed
6	Savanna, IL	Savanna Army Depot	Metals, Explosives, Solvents, VOCs/Aquatic	RI/FS, ERA Completed
7	Caddo Lake, TX	Longhorn Army Ammunition Plant	Explosives, Metals, VOCs/ Aquatic	RI/FS Completed
8	Chattanooga, TN	Volunteer Army Ammunition Plant	Aquatic	
9	West Point, NY	Army	Pb, Cu, Zn, Sb/Water, Plants, Fish/Aquatic/ Terrestrial	Planning
10	Joliet, IL	Joliet Army Ammunition Depot	Metals, PCBs, VOCs, PAHs, Solvents/Soil, Groundwater, Plants/ Aquatic/Terrestrial	RI Completed
11	Fort Lewis, WA	Army/R. Wilson	Pb, VOCs, PAHs, Solvents/Soil, Groundwater, Plants/ Terrestrial	ERA Completed
12	Kirtland AF Base, NM	Air Force/ M. Shuttlemore	Th/ Air, Soil, Surface Water/Terrestrial	RI Completed
13	Fort Jackson, SC	Army/G. Fabian	Pb/ Groundwater, Wetland/Aquatic	Preliminary Data
14	Point Mugu AWS, CA	Navy/K. Norris	Metals, VOC/Sediment, Water, Tissue/Aquatic/ Terrestrial	RI/FS, ERA Completed
15	Concord NWS, CA	Army/J. Canepa	Metals/Soil, Water, Plants, Tissue/Aquatic/Terrestrial	RI/FS, ERA Completed
16	Fort McCoy, WI	Army	White Phosphorus, Metals, Explosives/Soil, Water, Tissue/Aquatic/ Terrestrial	Preliminary Data
17	Pearl Harbor, HI	Navy	Metals, PAHs, Pesticides/ Sediment, Tissue/Aquatic/ Terrestrial	RI/FS Completed
18	Pueblo Army Depot	Army/ M. Anderson	TNT/Soil, Groundwater/ Terrestrial	RI/FS, ERA Completed
19	Twin Cities Army Ammunition Plant (SS)	Army/J. Moore (New Brighton)/ Arden Hills (SS)	Pb/Soil, Water/Aquatic/ Terrestrial	RI, EA Completed
20	Langley AF Base	Air Force/ J. Moore	Metals, TCE, Pesticides/ Water, Sediment/Aquatic	RI and EA Completed
21	FE Warren AF Base	Air Force/ K. Englert	Metals, Pesticides, VOCs, PCBs	RI Completed

RI = Remedial Investigation  
 FS = Feasibility Study  
 ERA = Ecological Risk Assessment  
 SS = Superfund Site  
 EA = Ecological Assessment  
 POC = Point of Contact

The advantages of selecting the LAFB site for this study included:

- CSM was presented.
- Food and Drug Administration (FDA) limits and risk-based screening levels (RBSLs) were used.
- An ERA and an HHRA were completed.
- Risk Assessment Guidelines for Superfund (RAGS) documentation is provided.
- All sediment, water, and animal tissue data were reported.
- Historical data are available to calculate future risks.
- Fate and transport information was provided.

## Pueblo Chemical Depot

Earth Tech (2002) summarized the SERA conducted at PCD. The selected site is the TNT Washout Facility and Discharge System (SWMU 17) located within a short-grass prairie community and adjacent to an open-water area. More information about the site is given in Chapter 5.

Advantages of selecting the PCD site for this study included:

- CSM was presented.
- Benchmark values were provided.
- SERA was completed.
- It was a small study area with a clearly defined source.
- It is an Army site.
- The site was contaminated with HMX and TNT (MRCs).

# 3 Model Description

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ARAMS has several computational modules for ecological risk evaluations that were used in the demonstrations. A brief description of these modules and some of the formulations are provided in this chapter.

## Aquatic Databases and Models

### Environmental Residue-Effects Database (ERED)

ERED (<http://www.el.erdc.usace.army.mil/ered>) is a Web-based residue-effects database for aquatic organisms. It is a compilation of organism toxicity effects information for contaminants of potential environmental concern. ERED is used in ARAMS to obtain aquatic ecological effects benchmarks to use in comparison to either measured or computed organism body burdens (i.e., tissue residues) to obtain an EHQ. For each organism and constituent (chemical or contaminant) combination selected, for which there are data, ERED provides information on the body part affected (e.g., whole body, stomach, etc.), the type of effect (e.g., lowest observable effects dose, LOED; no observable effects dose, NOED; effects dose that affected 50 percent of test subjects, ED50, etc.), the effect observed (e.g., mortality, growth, etc.), the measured body burden that produced the effect (mg/kg wet), and the duration of the tests that produced the effect.

A data-client editor (DCE) was developed for ARAMS that allows the user to conduct queries of the on-line ERED, retrieve data, and store the retrieved data in a FRAMES global input data (GID) file for use in the ARAMS application. The ERED DCE queries can be performed in a seamless fashion. The constituents are selected within the constituent database and passed to the ERED DCE. ARAMS also has Terrestrial and Aquatic Organism Selectors (TOS and AOS, respectively) that are used to select organisms, and these selections are passed to the Aquatic Benchmark Object (e.g., ERED) and other objects. Other objects can access the retrieved aquatic toxicity benchmarks from ERED, such as the Eco Health Effects Object for calculating EHQ. The only module in the Eco Effects Object is the Wildlife Ecological Assessment Program (WEAP), which is described below.

All available data for constituent and organism combinations can be retrieved for viewing and editing. Each selected organism is assumed to be associated with each COC, forming  $c \times s$  pairs for retrieval, where  $c$  is the number of

constituents, and  $s$  is the number of species (organisms). Although the database is the result of an extensive literature search of known residue-effects data, the database still has many data gaps considering the large number of species and chemical compounds in existence. The database is updated annually as new information becomes available.

Alternative approaches may be considered for evaluating the potential for biological effects associated with a particular residue level when the database contains either limited or no data for a specific compound or organism. One such approach, referred to as the critical body residue (CBR), enables researchers to make use of residue-effects information for compounds acting by the same mode of action as the compound for which data are not available (see McCarty et al. 1992 and McCarty and Mackay 1993).

At the time of this report preparation, the ERED contained data from 736 studies published between 1964 and 2001. From those studies, 3,463 distinct observations were included on-line. The ERED includes data on 222 analytes, 188 species, 13 effect classes, and 126 endpoints. Most papers involving mixtures of contaminants were excluded from the database because effects could not be linked to a specific constituent.

The ERED DCE allows the user to alias target constituents and organisms to those constituents/organisms for which there are data in the ERED. The DCE defaults to aliasing constituents and organisms to their respective selves. However, as mentioned previously, there may be instances where a constituent of concern or where a target organism is not in the ERED. In these situations, users must supply their own data for the constituent/organism pair or alias the constituent/organism to a similar constituent/organism that is in the ERED. The ERED DCE has a tree-view tool located on the “Constituents/Organism Aliasing” tab that allows the users to see what constituents/organism pairs have data in the ERED. After selecting any aliases that may be required, users can retrieve the data from the ERED by clicking the “Retrieve Data” button. This will query the ERED and then display any results on the “Select Data for Downstream Modules” tab. The users should select the data that they wish to use in the analysis by selecting the “SendData” checkbox button located beside the data. If there are no data for a given constituent/organism pair, then that row of data will be incomplete, but the user can then click on the row, which launches an input screen to enter user-defined residue-effects data.

### **Biota/Sediment Accumulation Factor (BSAF) Database**

BSAF is used commonly to calculate aquatic tissue residue associated with contaminated bottom sediments, especially for benthic organisms. BSAF has exactly the same meaning as pf (preference factor), AF (accumulation factor), or PF (partitioning factor) used in earlier literature. The BSAF Database contains bioaccumulation factors (BAFs) and lipid data for specified pairs of aquatic organisms and constituents (chemicals) of concern. Empirically derived BSAF values are calculated as:

$$\text{BSAF} = (C_t / f_L) / (C_s / f_{oc}) \quad (1)$$

The numerator of the above equation is the lipid-normalized constituent concentration in the tissue of the exposed organism, and the denominator is the organic carbon-normalized contaminant concentration in the sediment to which the organism has been exposed. Variables in Equation 1 are defined as

$C_t$  = constituent concentration in organism tissue, mg/kg wet weight

$f_L$  = organism's lipid fraction by wet weight

$C_s$  = constituent concentration in sediment, mg/kg

$f_{oc}$  = sediment organic carbon fraction by weight

Care must be exercised to ensure that wet and dry weights are used appropriately. Sediment concentrations are usually reported on a dry weight basis; in those cases,  $f_{oc}$  should also be in dry weight (which usually is the case). ERED tissue residues are reported in wet weight; it is beneficial to obtain  $C_t$  in weight wet for calculation of EHQ, so lipid fractions should also be in wet weight.

BSAFs are retrieved for organisms of concern and target constituents. The lipid data are retrieved for only target organisms. The query displays individual records and the resulting query mean, standard error, and range summary information. BSAF is used to provide information to the theoretical bioaccumulation potential (TBP) model described below.

## RECOVERY

RECOVERY is a surface water model in ARAMS/Frames that may be used to simulate the time-varying fate and concentration of contaminants (in the water column and in sediment bed) resulting from initial contamination and external contaminant loadings. The system is idealized as a well-mixed water column with a mixed surficial sediment bed layer underlain by a vertical stratified sediment column. The sediment is segmented into the well-mixed surface layer and deep sediment for model inputs and numerical solution. The deep sediment can consist of contaminated and uncontaminated regions with varying levels of contamination and varying sediment properties. RECOVERY utilizes reversible, linear, equilibrium partitioning of contaminant between sediment solids and water, volatilization, and first-order contaminant degradation. Flow through the water body is assumed to be constant (Ruiz and Gerald 2001). Sediment concentrations computed by RECOVERY are converted from mass chemical/total volume of sediment and water to mass chemical/mass sediment (dry) for output and use with other modules in Frames.

## User-Defined Eco Body Burden Module (Known BBF)

The purpose of the known body burden concentration file (Known BBF) module is to allow the user to input user-defined aquatic organism body burdens (i.e., tissue residues, mg chemical/kg organism body wet weight) to provide the

appropriate data that can be used by other modules, e.g., Eco Effects. This module is used only if the body burden concentrations are known. The chemical body burden concentrations are entered directly through the module user interface (MUI). Both radionuclides and other chemicals can be input into this module. The constituent concentrations are time varying, and the user defines the time points. If tissue residue data are available for only one time point, then two time points must be entered, but the values at the second time point can be the same as those at the first, which would result in a steady-state analysis.

### Theoretical Bioaccumulation Potential (TBP) Model

The TBP Model uses equilibrium partitioning of contaminants in sediments to organisms. TBP assumes a closed system consisting of sediment, organism, and water. A neutral organic chemical in the system is given free movement and will distribute throughout the phases in contact until a condition of equilibrium is established. The concentrations at equilibrium are determined by chemical potential in each phase. Organic carbon in the sediment and lipid in the organism are assumed to be the primary compartments that account for partitioning of neutral chemicals. Thus, the concentration of a chemical in the sediment is normalized on the basis of its organic carbon content, and the application of a partition coefficient (i.e., BSAF) enables calculation of the expected equilibrium concentration in an exposed organism of stated lipid content (McFarland 1984, McFarland and Clarke 1986).

TBP estimates tissue concentration (or tissue residue), TC (mg/kg), based on Equation 1:

$$TC = BSAF(C_s / f_{oc})f_L \quad (2)$$

In the above equation, the consistent concentration of wet or dry weight units should be used. If  $C_s$  is in dry weight, then  $f_{oc}$  should be expressed in terms of dry weight fraction. Similarly, if TC is desired in wet weight, which is the case in ARAMS/FRAMES for use by other modules, then  $f_L$  should also be in terms of weight wet fraction.

### TrophicTrace Model

TrophicTrace is a tool for assessing risks from trophic transfer of sediment-associated contaminants (<http://el.erdc.usace.army.mil/trophictrace/index.html>). TrophicTrace is a Microsoft Excel program for calculating the potential human health and ecological risks associated with bioaccumulation of contaminants in sediments. More details are available in von Stackelberg and Bridges (2002), which provides a management guide with quantitative examples.

TrophicTrace is a stand-alone model with ARAMS, which means it presently does not link with any other models or modules. The reason for this is that TrophicTrace was designed to provide the complete analysis of exposure and effects, whereas all the modules that can be linked within FRAMES were

designed to provide a specific function, such as calculate tissue residue, as in TBP.

The TrophicTrace main screen input menu is divided into the following data options: Chemicals, Environment, Invertebrates, Fish, Human Exposure, Mammals, Avian, Create Output, and Help. Several of these options are described below.

TrophicTrace uses the Gobas (1993) steady-state uptake model to estimate fish body burdens (concentration in fish) for hydrophobic organic compounds (von Stackelberg and Burmistrova 2003) as:

$$C_f = \frac{k_l * C_{wd} + k_d * C_{diet}}{k_2 + k_e + k_m + k_g} \quad (3)$$

where

$C_f$  = concentration in fish, mg/kg

$k_l$  = gill uptake rate, L/kg/d

$C_{wd}$  = dissolved concentration in water, ng/L

$k_d$  = dietary uptake rate, d<sup>-1</sup>

$C_{diet}$  = concentration in diet, µg/kg

$k_2$  = gill elimination rate, d<sup>-1</sup>

$k_e$  = fecal ingestion rate, d<sup>-1</sup>

$k_m$  = metabolic rate, d<sup>-1</sup>

$k_g$  = growth rate, d<sup>-1</sup>

The report by von Stackelberg and Bridges (2002) provides equations to estimate the rate constants ( $k_2$ ,  $k_e$ ,  $k_m$ , and  $k_g$ ). If the metabolic rate,  $k_m$ , is small compared to  $k_2$  or  $k_e$ , then its value becomes irrelevant and  $k_m$  can be assumed to be zero (Gobas 1993).

TrophicTrace includes data for several fish receptors. For example, a mid-trophic level fish consumes benthic invertebrates, and an upper trophic level fish consumes the mid-trophic level fish. Subsequently, the upper trophic level fish may be consumed by a piscivorous bird such as belted kingfisher or carnivorous mammal such as mink.

The food web model for birds (avian) is given as:

$$\text{Dose Concentration (bird)} = \frac{(C_w * WI) + (C_{fish} * FI * F_{fish}) + (C_{crab} * FI * F_{crab})}{BW} * GI \quad (4)$$

where

$C_w$  = water concentration, mg/L

*WI* = water intake rate, L/day

*C<sub>fish</sub>* = concentration of COPEC (see Appendix A) in fish, mg/kg

*FI* = food ingestion rate, kg/day

*F<sub>fish</sub>* = dietary fraction of fish, unitless

*C<sub>crab</sub>* = concentration of COPEC in crabs, mg/kg

*F<sub>crab</sub>* = dietary fraction of crabs, unitless

*BW* = body weight, kg

*GI* = gastrointestinal absorption factor, unitless

The GI in the food web models is used for the baseline ecological risk assessment (BERA). For the SERA, GI is equal to 1.

The food web model for mammal is given as:

$$\text{Dose Concentration (mammal)} = \frac{(C_w * WI) + (C_{fish} * FI * F_{fish}) + (C_{bi} * FI * F_{bi})}{BW} * GI \quad (5)$$

where

*C<sub>bi</sub>* = concentration of COPEC in benthic invertebrates, mg/kg

*F<sub>bi</sub>* = dietary fraction of benthic invertebrates, unitless

Other parameters were defined previously.

TrophicTrace uses trapezoidal fuzzy numbers to characterize parameter uncertainty. A trapezoidal fuzzy number is simply four numerical values (A, B, C, D) where A ≤ B ≤ C ≤ D. The number A is the minimum possible value of the parameter, and D is the maximum possible value of the parameter. The range [B,C] is the most likely range of the parameter. Fuzzy results yield both “worst case” and “best estimates” simultaneously (von Stackelberg and Burmistrova 2003). Through the use of fuzzy numbers, TrophicTrace output provides four estimates instead of one.

Estimates of fish body burdens for inorganic and hydrophilic organic chemicals rely on two approaches, depending on data availability. The first approach is a trophic transfer factor (TTF), and the second is the bioconcentration factor (BCF) approach. For some chemicals, there are data available on bioaccumulation from invertebrates to fish (Dillon et al. 1995). TTF is used to compute predator (e.g., fish) concentration given prey concentration, such as benthic invertebrates, both in wet weight concentration units (mg/kg). TTF values are based on regression of data from studies of predator-prey ratios. Currently, TTF values are available for arsenic, copper, cadmium, lead, and zinc. In the BCF approach, water concentrations are multiplied by a bioconcentration factor to estimate fish body burdens. Water concentrations can either be provided by the user or estimated by the model assuming equilibrium partitioning from sediment.

## **Wildlife Ecological Assessment Program (WEAP)**

WEAP (Whelan et al. 2000) is an updated version of the FFrequency ANalysis of COncentration (FRANCO) model, which was developed by PNNL for the USEPA for regulatory and compliance purposes. The options in WEAP will change and be available according to the upstream modules that are connected to WEAP. WEAP is a statistical package that (a) correlates duration of exposure to contaminant levels to help determine the impacts of the exposure to organisms and (b) bridges the gap between simulated chemical fate/transport modeling and ERA data that are available from laboratory studies. The WEAP statistical analysis accommodates different organisms as they relate to different contaminants, resulting in a flexible and versatile tool.

WEAP analyzes time-varying water-column concentrations and compares these results to ecological benchmarks to determine health impacts to selected life forms. WEAP tabularizes the percentage of time that a life form is associated with an ecological health impact region for a given chemical, based on (a) time-varying water-column concentrations, (b) an impact-toxicity benchmark curve (e.g., percent mortality for a lethal concentration, i.e., a LC curve), and (c) a lower acceptable limit curve. WEAP also computes EHQs based on the ratio of organism dose (tissue residue for aquatic organisms) to toxicity reference value (TRV) (effects tissue concentration for aquatic organisms) and determines cumulative probabilities of exceeding various EHQ levels based on time-series data of EHQ.

In ARAMS/FRAMES, the WEAP module may be connected to: modules that produce a surface water concentration file (WCF), the Eco Tissue Concentrations module that produces a BBF in units of mg/kg (wet), and to an Eco Receptor Intake module that produces a terrestrial wildlife intake (TWI) file in units of dose (mg/kg/day). WEAP should also be connected to aquatic and terrestrial eco benchmark modules that provide effects benchmarks for computing EHQs.

WEAP compares simulated or measured ecological constituent (i.e., chemical of concern) levels (e.g., media concentration, receptor body burden, or receptor dose) with TRVs to obtain EHQ, i.e., EHQ = eco level / TRV. WEAP also provides other information, such as percentage of time that an organism incurs an effect based on time-varying concentrations or doses.

WEAP produces basic types of output for time-varying concentrations, doses, or body burdens. The forms of outputs are described as follows:

- a. When consuming information from a WCF, WEAP produces a table and chart of acute (e.g., 96-hr) and chronic exposures (e.g., >96-hr) with percentage of time that a time-series of concentrations is:
  - (1) Below an acceptable limit (e.g., chronic limit, criterion continuous concentration [CCC], no observable effects level [NOEL], no observable adverse effects level [NOAEL], etc.).
  - (2) Above an unacceptable limit (e.g., exposure duration curves associated with lethal concentration for 50 percent mortality

[LC-50], lethal dose for 50 percent mortality [LD-50], effective dose at 50 percent [ED-50], etc.).

- (3) In between acceptable and unacceptable limits. This table results in a maximum of six values.
- b. When consuming information from a WCF, WEAP produces a table and graph reporting the probability of exceedence (based on cumulative frequency analysis of time-series data) versus concentration, i.e., the probability that concentration will be equal to or greater than a selected value.
- c. When consuming a BBF or TWI file, along with the ecological effects benchmarks, WEAP produces a table and graph reporting EHQ versus time. EHQ is defined as the ratio of tissue residue concentration to benchmark effects residue concentration for aquatic organisms, or daily dose to a benchmark dose for terrestrial organisms, i.e.,

$$EHQ = \frac{\text{Concentration of Chemical in Tissue}}{\text{Critical Effect Concentration}} \quad (6)$$

$$EHQ = \frac{\text{Total Daily Dose}}{\text{TRV}} \quad (7)$$

- d. When consuming a BBF and TWI, WEAP produces a table and graph reporting probability of exceedence (based on cumulative frequency analysis of time-series data) versus EHQ, i.e., probability that an EHQ will be equal to or greater than a selected value. WEAP also produces a table and graph reporting probability of exceedence versus dose or body burden, i.e., probability that the dose/body burden will be equal to or greater than a given value.

## Terrestrial Databases and Models

### Terrestrial Toxicity Database (TTD)

The TTD (Wirtz and Fairbrother 2001) provides a selection of ecologically relevant TRVs for wildlife and soil screening-level (SSL) benchmarks for plants and soil invertebrates. The database was developed by reviewing values derived by various jurisdictions (i.e., regulatory or promulgation entities) and ranking them according to quality and relevance. The ranked values are supplied in a Microsoft Access 2000 database that is searchable by genus, family, order, class, general data groupings (e.g., all soil benchmark values), chemical name, or Chemical Abstracts Service Registration Number (CAS Number) or synonym. The default value is the most conservative TRV or benchmark value with the highest quality ranking and thus, total score; however, a user may select another value deemed of lesser quality if desired. After a thorough evaluation of applicable data from a wide range of jurisdictions, a total of 1,156 TRVs/benchmarks from 10 different jurisdictions were included in the database. The TRVs/benchmarks represent data on 315 chemicals. TRVs are available for the

classes of Amphibia, Aves, and Mammalia. At the time of this study, TTD did not have data for Reptilia. Therefore, if this option is selected, “No Data Available” appears on the screen. SSL benchmarks are available for the five general data groupings of Soil, Soil/Earthworms, Soil/Invertebrates, Soil/Plants, and Soil/Plants/Invertebrates.

The TTD DCE in ARAMS/FRAMES allows the user to select terrestrial organism TRVs and SSLs for the constituents of concern selected in the constituent database module. Constituents of concern and target organisms are passed to the TTD DCE from the Constituent Database editor and Terrestrial Organism Selector, respectively. The SSLs are dependent only on the constituents selected. The basic operating procedure for the DCE is to press the “Submit Query” button located on the “Chemicals” tab. After retrieving data available in the database for the constituents of interest, the users can view select which TRVs or SSLs to use in their analysis. User-defined SSLs and TRVs can also be entered. The TTD DCE also allows aliasing similar to the ERED and BSAF DCEs.

### **Terrestrial Wildlife Exposure Model (TWEM)**

TWEM (USACHPPM 2004) estimates oral exposure levels (mg/kg/day) for terrestrial wildlife through ingestion of water, soil, sediment, and food items. Output from TWEM is used with TRVs for EHQ calculations. TWEM accepts abiotic media concentration data (soil, sediment, and water concentrations in units of mg/kg, mg/kg, and mg/L, respectively) from other ARAMS modules and uses these to compute media doses and food concentrations and doses. TWEM links the concentration data with bioaccumulation models from the client-machine-based, chemical-specific bioaccumulation factor (BAF, mg chemical/kg food item/mg chemical/kg soil) database that was developed for TWEM to produce estimated chemical concentrations (mg/kg wet weight) in different food types.

Chemical oral exposure estimates (doses, mg/kg/day) are obtained from

$$E_j = \left[ \left( Soil_j \times P_s \times FIR \right) + \left[ \sum_{i=1}^N \left( B_{ij} \times P_i \times FIR \right) \right] + \left( Water_j \times WIR \right) \right] \times AUF \quad (8)$$

where

$E_j$  = total exposure (dose) to chemical  $j$ , mg/kg/d

$Soil_j$  = concentration of chemical  $j$  in soil and/or sediment, mg/kg

$P_s$  = soil proportion of diet, fraction, dimensionless

$FIR$  = species-specific food ingestion rate, kg food/kg body weight/d

$N$  = number of food items

$B_{ij}$  = concentration of chemical  $j$  in biota type  $I$ , mg/kg

$P_i$  = proportion of biota type  $i$  in diet, fraction, dimensionless

$Water_j$  = concentration of chemical  $j$  in water, mg/L

$WIR$  = species-specific water ingestion rate, L/kg (body weight)/d

$AUF$  = area foraging factor, calculated as the contaminated site area divided by the species home range, fraction, value cannot exceed 1.0

Output from TWEM is consumed by WEAP in the Eco Effects Object to produce EHQ values. Although the TWEM output file for FRAMES (TWI) is assumed to be time varying, TWEM can presently function as only a single event (single time point) model. Thus, all values in the TWI file are constant over time. It is possible to extend TWEM in the future to include time-varying exposure values as well as dermal and inhalation exposure as additional exposure and effects information becomes available. Presently, TWEM finds the largest media concentrations in the incoming files, and uses those for its calculations.

It is important to recognize that TWEM is not a spatially explicit exposure model, i.e., receptors are assumed to always be exposed to contamination even if their home range is larger than the contaminated area, which is a highly conservative approach. Spatially explicit models, such as the Spatially Explicit Exposure Model (SEEM) (Wickwire et al. 2004), provide a more realistic estimate of exposure since the level of contamination and habitat quality can vary over a spatial grid, and the receptors can move or forage over the grid.

TWEM has a Life History Database for providing receptor body weight, home range area, food and water ingestion rates, diet, and soil or sediment fractions as proportion of diet. As mentioned above, TWEM also has a BAF Database for use in estimating food concentrations. This database has chemical-specific parameters for three models: regression models, BAF models, and Log  $K_{ow}$  models. Regression models use media concentrations within a regression equation to estimate food item concentrations. BAF models multiply the media concentration by the BAF value to estimate the food item concentration. Log  $K_{ow}$  models are regressions that estimate food item concentration based on the media concentration and the Log  $K_{ow}$  value. Of course, the database is fairly sparse since parameters are not available for all three models for each food item and each chemical. TWEM allows the user to select from each available model, use a rule-based estimate, or use measured food concentrations. The rule-based estimate will use whatever is available in the database with this hierarchical order: regression model, BAF model, Log  $L_{ow}$  model, or BAF model with BAF = 1.0 if the other models are not available.

Food and water consumption rates that are needed for TWEM are obtained from the Life History Data. Values in the database may have been reported in the literature or calculated for each receptor species using Nagy's (1987) allometric equations as reported in the "Wildlife Exposure Factors Handbook" (USEPA 1993). The equations correlate food and water intake to body weight in free-living wildlife species. Separate food regression equations are used for mammals, birds, and herpetofauna. Calder and Braun (1983), as cited in the "Wildlife Exposure Factors Handbook" (USEPA 1993), developed equations for drinking water ingestion for birds and mammals. No similar allometric equation is available for relating body weight to drinking water ingestion for reptiles and

amphibians. Therefore, a default value of 0.0001 is used for water ingestion in all herpetofauna.

### **Conceptual Site Model (CSM)**

A CSM is an integral part of a site investigation and/or ERA as it provides the framework from which the study design is structured. The CSM follows contaminants from their sources, through transport and fate pathways (air, soil, surface water, groundwater), to the ecological receptors and is normally shown by a flowchart. The CSM is a strong tool in the development of a representative sampling plan and is a requirement when conducting an ERA. It assists in evaluating the interaction of different site features (e.g., drainage systems and the surrounding topography), thereby ensuring that contaminant sources, pathways, and ecological or human receptors throughout the site have been considered before sampling locations, techniques, and media are chosen.

ARAMS has a CSM development tool that through a series of interactive screen queries helps the user development features of the CSM. Following the queries, the system automatically generates the CMS diagram and Table 1 of RAGS for human health assessments.

## 4 Aquatic Site

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### Langley Air Force Base Site

The site for the aquatic ecological demonstration is located at Langley Air Force Base (LAFB). LAFB occupies 3,152 acres<sup>1</sup> near Hampton, VA (URS Corporation 2002a, 2002b). LAFB and the National Aeronautics and Space Administration (NASA) Langley Research Center form a peninsula, which divides the Back River into northwest and southwest branches (Figure 1). The Back River is a tidal estuary of Chesapeake Bay. Five major investigations have been performed to characterize contamination or water quality in the Back River. In addition to LAFB and NASA, significant areas of residential and commercial development exist in the nearby area. Contaminants are transported to Back River by point source and non-point source discharges. Contaminants include PAHs (polycyclic aromatic hydrocarbons), PCBs (polychlorinated biphenyl)/PCTs (polychlorinated terphenyls), pesticides, and metals. Wetlands such as Plum Tree Island National Wildlife Refuge and submerged aquatic vegetation provide important nursery and feeding habitat for a variety of fish species and shellfish (URS Corporation 2002a).

URS Corporation (2002a), under a contract to LAFB, conducted a site ERA. The report includes a detailed characterization of the exposure pathways for benthic invertebrates, Atlantic croaker, belted kingfisher, and mink. Mink and belted kingfisher are classified as semi-aquatic species. For example, fish and shellfish were identified as the primary and secondary food sources for the kingfisher, respectively.

Among the contaminants at the site, PCB (Aroclor 1254), benzo(a)pyrene, and arsenic were selected for this demonstration. PCBs can bioconcentrate, bioaccumulate, and biomagnify in aquatic environments. Reported BCFs for freshwater invertebrates exposed to PCB range from 60 to 27,000 (unitless). URS Corporation (2002a) indicated that diet is the major route of PCB uptake in freshwater fish. Aquatic invertebrates normally contribute to the cycling of PCBs. The biomagnification in the aquatic environment results from resistance of highly chlorinated congeners to metabolize and the high affinity of PCBs for lipids (URS Corporation 2002a). In the terrestrial environment, PCBs are detected more frequently in mammals and birds than in plants. PCBs are readily absorbed through the gastrointestinal tract and skin. Exposure of vertebrates to PCBs can induce the production of mixed-function oxidase enzymes that

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<sup>1</sup> A table of factors for converting U.S. customary units to metric (SI) is presented on page vi.

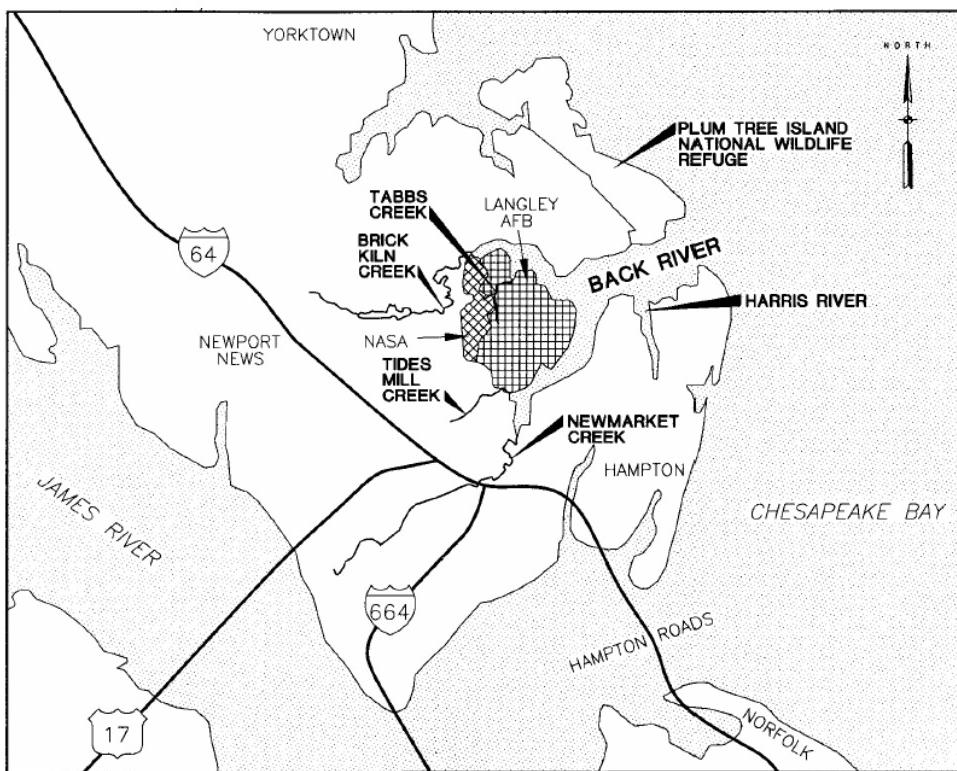


Figure 1. Location map of Langley Air Force Base, Virginia

metabolize foreign compounds. PCB metabolites may be more toxic than the parent compound. Minks are especially sensitive to PCB contaminations (URS Corporation 2002b).

Benzo(a)pyrene is classified as a PAH. PAHs are a diverse group of organic chemicals consisting of substituted and un-substituted polycyclic and heterocyclic aromatic rings. PAHs are formed as a result of incomplete combustion of organic materials such as wood, coal, and oil. Approximately 270,000 metric tons of PAHs reach the environment annually. PAHs are accumulated in terrestrial and aquatic plants, fish, and invertebrates. However, many animals are able to metabolize and eliminate these compounds from their system. For aquatic organisms, PAHs in the molecular range from naphthalene to pyrene are considered acutely toxic. There is evidence to suggest that PAHs are responsible for the reproductive and teratogenic effects in eggs, delayed hatch, and gross abnormalities. Benthic organisms obtain a majority of their PAHs from sediments through their ability to mobilize PAHs from the sediment/pore water matrix. The elevated levels in benthic organisms could provide a significant source of PAHs to predatory fish. However, fish have the ability to metabolize and degrade PAHs (URS Corporation 2002b).

Arsenic occurs naturally as sulfides and is present in rocks, soils, water, and living organisms at parts-per-million concentrations. Arsenic also occurs as complex sulfides of iron, nickel, and cobalt and is constantly being oxidized, reduced, or otherwise metabolized. In general, the inorganic arsenic forms are more toxic to aquatic wildlife than the organic forms, and trivalent species are

more toxic than the pentavalent species. This demonstration assumes inorganic arsenic as one the contaminants of concern at the site. Arsenic toxicity and other effects to aquatic life are significantly modified by numerous biological and abiotic factors. These factors include water temperature, pH, Eh, organic content, suspended solids, duration of exposure, and the presence of other toxicants (URS Corporation 2002b).

## ARAMS Application

Several modules of ARAMS were used to estimate aquatic ecological risks to the four selected assessment endpoints, which included benthic invertebrates, Atlantic croaker, belted kingfisher, and mink. Actually, the belted kingfisher and mink can be considered as terrestrial organisms, and their exposure can be modeled with TWEM. Data are available in the TWEM databases for these two organisms. However, for this aquatic demonstration, it seemed more appropriate to use modules that were developed for such assessments; thus, TWEM is not used in this example. Instead, TrophicTrace is used to compute exposure and risks for the Atlantic croaker, belted kingfisher, and mink. TWEM will be used in the terrestrial ERA demonstration. Both the Known BBF and TBP modules were used to input/estimate tissue residues for benthic invertebrates, and WEAP was used to compute risks. The TBP-WEAP approach used the RECOVERY fate and transport model to obtain water and sediment concentrations. TBP is not appropriate for computing tissue residue for the fish, bird, and mink, nor does it compute oral exposure dose like TWEM does. Thus, the TrophicTrace model was used since it does include fish uptake and oral exposure dose calculations. Additionally, TrophicTrace has the capacity to estimate risks to assessment endpoints using either measured or estimated diet tissue concentrations, which were included in this demonstration.

### Development of conceptual site model (CSM)

One conceptual site model (URS Corporation 2002a) includes primary and secondary sources of contaminants with four types of media (Figure 2). The ERA report, however, describes the use of a conceptual site model with only secondary sources of contaminants, which was utilized in this demonstration (Figure 3). The media of concern include water from the Back River, sediment, and aquatic/wetland prey. The risks quantified in this demonstration assumed the sediment was the source of contamination and ingestion was the exposure route.

### Benthic invertebrates

Two approaches of ARAMS and TrophicTrace were used to estimate risks to benthic invertebrates. The ARAMS/FRAMES/BBF-WEAP approach (Figure 4) is used when the body burden value is known. The ARAMS/FRAMES/TBP-WEAP approach (Figure 5) requires more site data, and body burdens are computed. For this application, a fate and transport model (RECOVERY) was used to provide computed sediment and water concentrations, although User-Defined

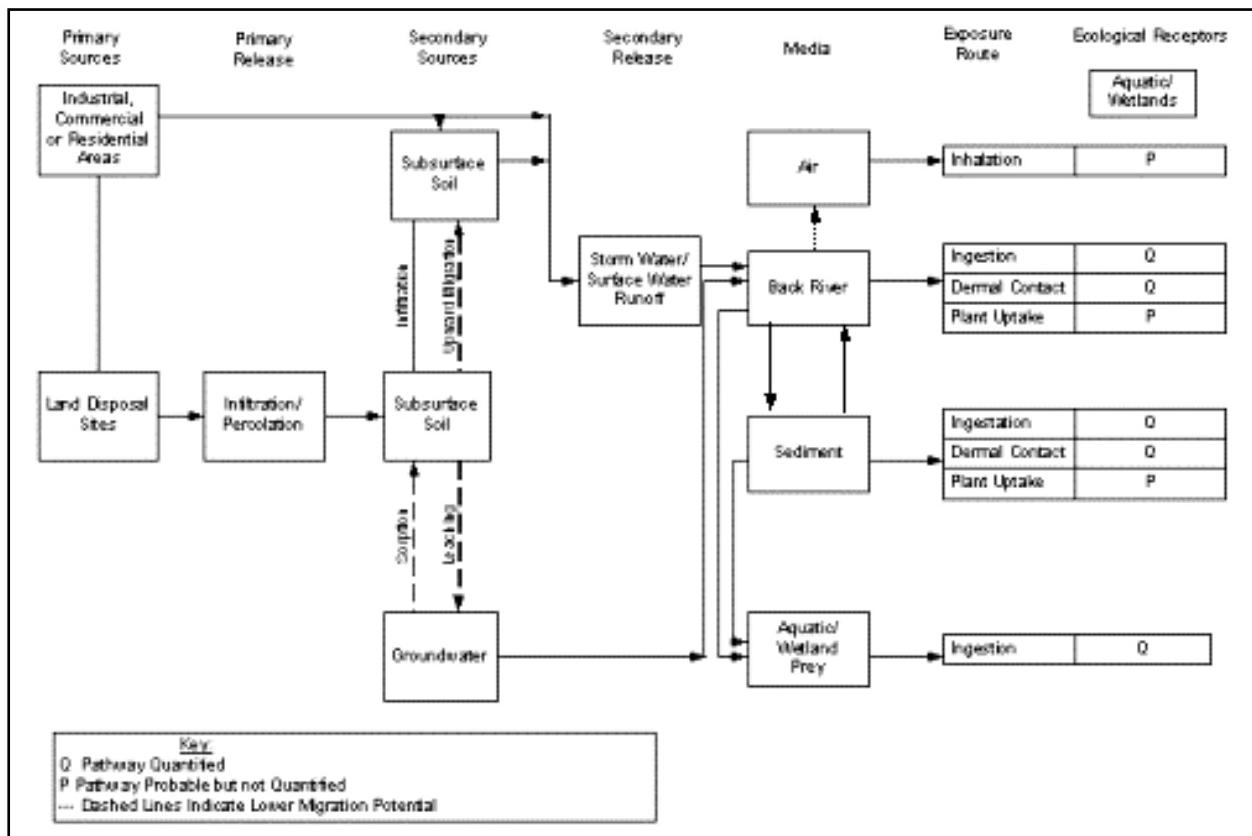


Figure 2. Possible ecological risk assessment conceptual model for Langley site (URS Corporation 2002a)

Known SCF and WCF modules could have been used for entering measured values. There was interest in knowing how well RECOVERY would perform for providing predicted concentrations. Inputs and results for both approaches (BBF-WEAP and TBP-WEAP) are presented.

Input data for the RECOVERY model for this application are shown in Table 2. The BSAF Database and DCE were used to select BSAF and lipid values for the chemicals and benthic invertebrates, which are used by TBP. Values of BSAF and percent lipid selected are shown in Table 3. The only input required for the TBP model, other than the sediment concentrations computed by the RECOVERY model, is the fraction of total organic carbon (TOC) in sediment by dry weight, which was set to 0.019 (Appendix C in the RI report, URS Corporation 2002b) for this application.

Table 4 provides the reported measured and computed tissue concentrations using TBP for benthic invertebrates. The computed tissue concentrations in Table 4 are for the initial sediment concentrations that were input to and output by RECOVERY to provide consistency with the measured tissue and sediment concentrations. As shown in Table 4, the computed tissue concentrations are very close to the measured values. The comparison is quite impressive given that there are three parameters that affect TBP result, which are BSAF, percent lipid, and sediment TOC, the first two of which were retrieved from the BSAF Database.

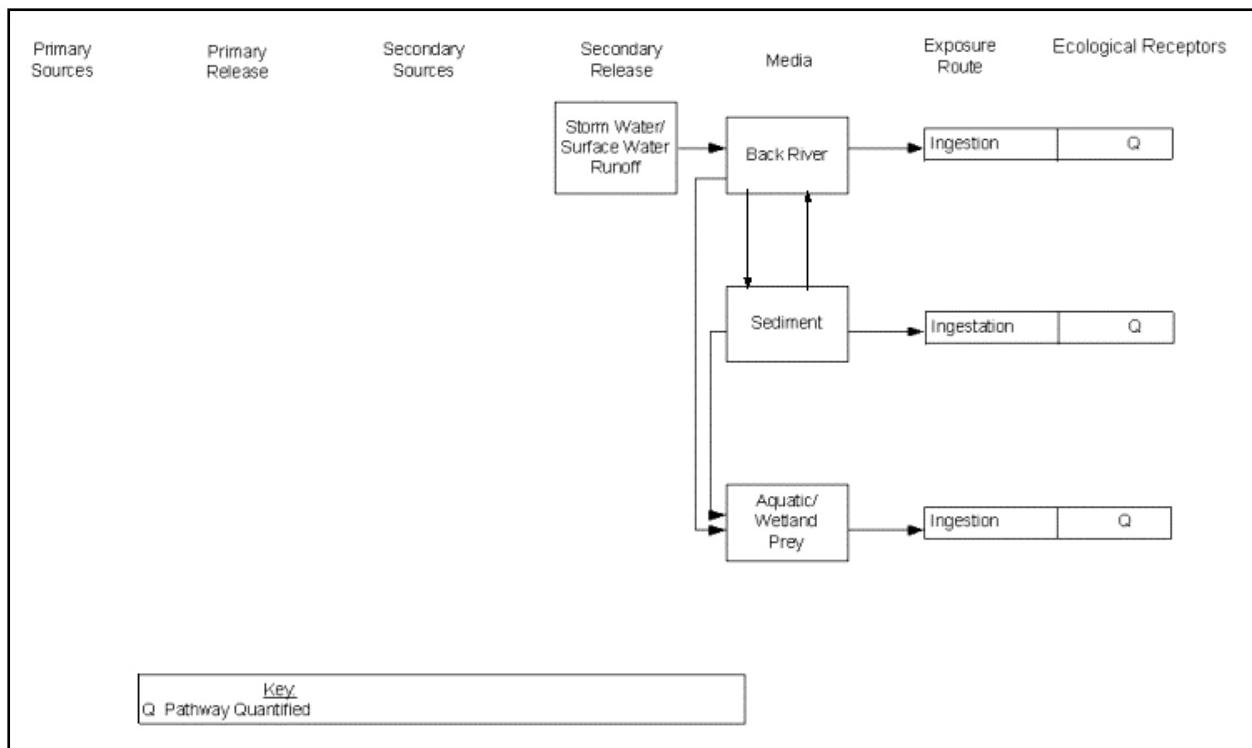


Figure 3. Langley CSM used in ARAMS/FRAMES demonstration

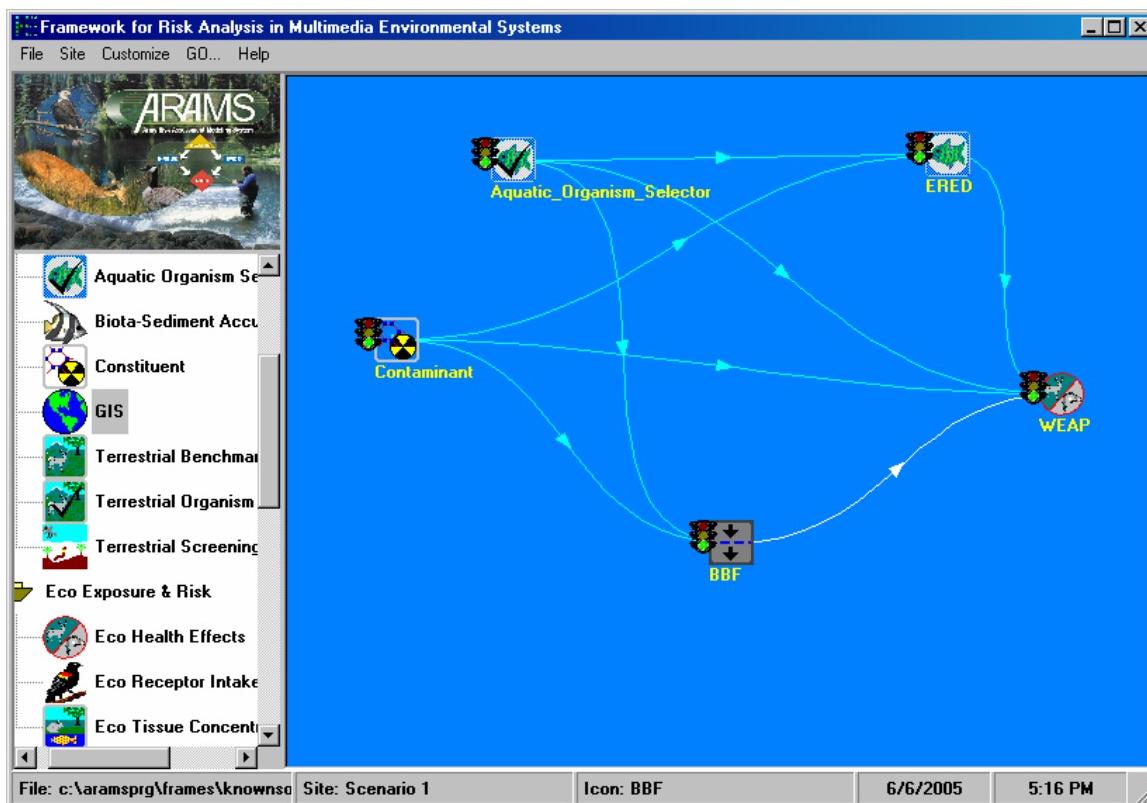


Figure 4. BBF-WEAP conceptual site model framework

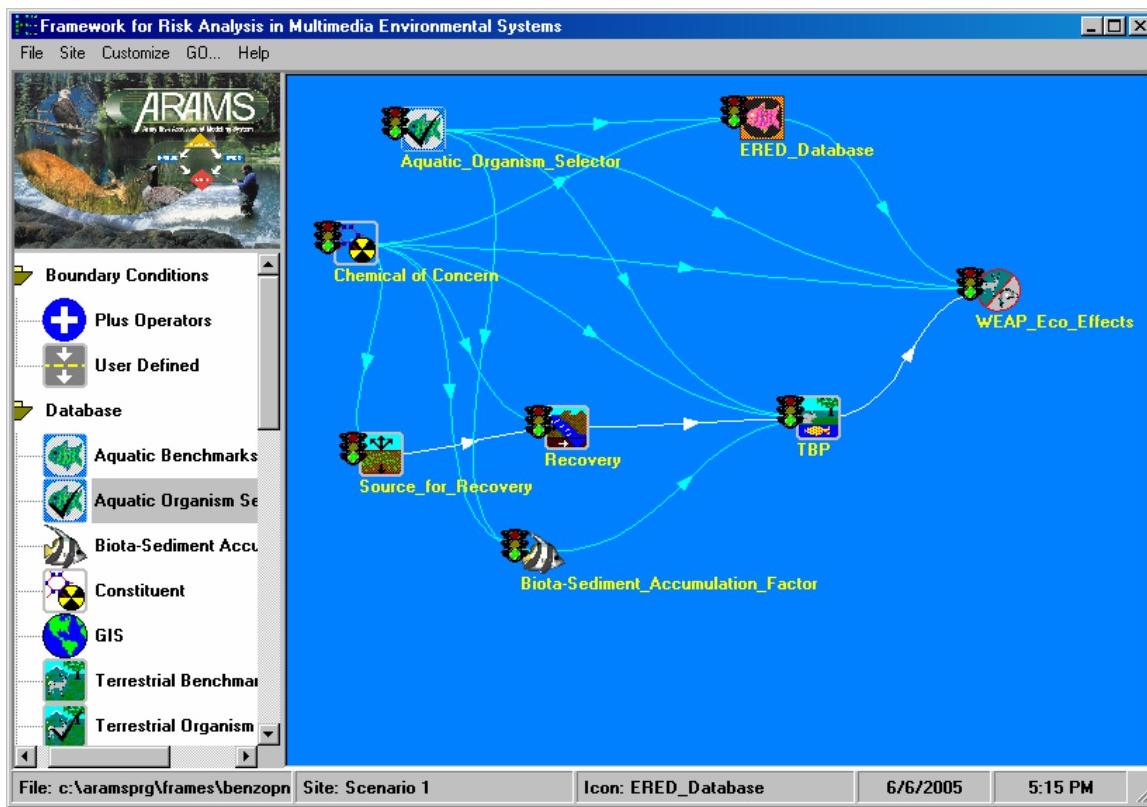


Figure 5. TBP-WEAP conceptual site model framework

TBP was developed for organic chemicals, so it was not used to calculate tissue residue for arsenic.

The reported TRV values based on NOAEL (Radian International LLC 1999) were used in the WEAP module as input (Table 5). The ERED Database and DCE did not have TRV values for these chemicals. The TBP-WEAP-computed and reported EHQ values are shown in Table 6 for comparison. The values compare closely since TBP produced fairly accurate tissue residues.

TrophicTrace also estimated the tissue residues for benthic invertebrates, and these results are shown in Table 4. The TrophicTrace tissue residues were also relatively close to the measured values for the organic chemicals and are identical to the values computed by TBP, which is reassuring since TrophicTrace uses the same equation as TBP (Equation 2) to estimate tissue concentrations of the diet of the ecological receptors. TrophicTrace uses the BCF parameter for inorganic chemicals multiplied by the water concentration to estimate tissue residues. Using a TrophicTrace default BCF of 3.5 L/kg for arsenic (USEPA 1999) and an observed dissolved in water concentration for arsenic of 3.74 µg/L resulted in a benthic invertebrate arsenic tissue concentration of 1.31E+01 µg/kg or 1.31E-02 mg/kg, which is far less than the measured value of 12.1. Clearly, a more appropriate BCF value is needed for arsenic.

**Table 2**  
**Langley Input Parameters for RECOVERY Input Data**

RECOVERY Source Term Model	PCB (Aroclor 1254)	Benzo(a)pyrene
Contaminant Initial Source Concentration in Water	0.0 µg/m <sup>3</sup>	0.0 µg/m <sup>3</sup>
Contaminant Inflow Concentration	(Assume zero) µg/m <sup>3</sup>	(Assume zero) µg/m <sup>3</sup>
Constant Contaminant External Load	0.0 kg/year	0.0 kg/year
<b>RECOVERY Water Body Model – Water Column</b>		
Suspended Solids Concentration	10 mg/L	10 mg/L
Weight Fraction Carbon in Solid	0.019 (no unit)	0.019 (no unit)
Surface Area	3,151,271 m <sup>2</sup>	3,151,271 m <sup>2</sup>
Depth	1.52 m	1.52 m
Annual Flow	94,610,000 m <sup>3</sup> /year	94,610,000 m <sup>3</sup> /year
Resident Time	(Assume zero) Computed	(Assume zero) Computed
<b>RECOVERY Water Body Model – Bed Mixed Sediment</b>		
Mixed Sediments Layer Depth	0.1 m	0.1 m
Contaminated Layer Depth	1.0 m	1.0 m
Mixed Layer Surface Area	3,151,271 m <sup>2</sup>	3,151,271 m <sup>2</sup>
Initial Concentration	1.21 mg/kg	9.314 mg/kg
Porosity	0.48	0.48
Particle Density	2,650,000 g/m <sup>3</sup>	2,650,000 g/m <sup>3</sup>
Weight Fraction Carbon in Solid *	0.019 (no unit)	0.019 (no unit)
<b>RECOVERY Water Body Model – Deep Contaminated Sediment Layer</b>		
Initial Concentration	4.18 mg/kg (Table H1-2)*	27.4 mg/kg (Table H1-2)*
Porosity	0.48	0.48
Particle Density	2,650,000 g/m <sup>3</sup>	2,650,000 g/m <sup>3</sup>
Weight Fraction Carbon in Solid *	0.1 (no unit)	0.1 (no unit)
<b>RECOVERY Water Body Model – System Properties</b>		
Wind Speed	High: 7.8 knots = 4.0 m/sec Low: 0.05 knot = 0.03 m/sec	High: 7.8 knots = 4.0 m/sec Low: 0.05 knot = 0.03 m/sec
Enhanced Diffusion	0.0 cm <sup>2</sup> /sec	0.0 cm <sup>2</sup> /sec
Enhanced Mixing Depth	(Assume zero)	(Assume zero)
Re-suspension Velocity	0.0 m/year (computed)	0.0 m/year (computed)
Burial Velocity	0.005 m/year	0.005 m/year
Settling Velocity	90 m/year	90 m/year
<b>RECOVERY Water Body Model – Chemical Properties</b>		
Henry's Constant	0.0083	2.45E-06
K <sub>ow</sub>	1.1E+06	9.33E+05
Decay Coefficient	(Assume zero)	(Assume zero)

\* Reference for Total Organic Carbon = Appendix C in RI Report (URS Corporation 2002b).

**Table 3**  
**Parameters Selected from BSAF Database for Benthic Invertebrates**

Chemical	BSAF (unitless)	Average % Lipid	Reference
Benzo(a)pyrene	1.7	1.06	von Stackelberg and Burmistrova (2003)
PCB (Aroclor 1254)	1.7	1.06	von Stackelberg and Burmistrova (2003)

**Table 4**  
**Measured and Estimated Tissue Concentrations for Benthic Invertebrates**

Contaminant	Measured (mg/kg wet), Langley RI <sup>1</sup> Report	Computed (mg/kg wet)	
		TBP	TrophicTrace
Benzo(a)pyrene	2.74E+01	2.60E+01	2.60E+01
PCB (Aroclor 1254)	4.18E+00	3.96E+00	3.96E+00
Arsenic	1.21E+01	NA <sup>2</sup>	1.31E-02 <sup>3</sup>

<sup>1</sup> Appendix H1-1 (URS Corporation 2002b).  
<sup>2</sup> NA = Not applicable (see discussion in text).  
<sup>3</sup> BCF method used.

**Table 5**  
**TRV Values (NOAEL-Based) for Benthic Invertebrates**

Contaminant	NOAEL (mg/kg)	Reference
Benzo(a)pyrene	1.20E+00	Radian International LLC (1999)
PCB (Aroclor 1254)	1.00E-02	Radian International LLC (1999)
Arsenic	8.50E+00	Radian International LLC (1999)

The Known BBF module allows the input of known tissue residue concentration for use by other modules. The measured tissue concentrations shown in Table 4 were used to populate the Known BBF input screen. The calculated EHQ values obtained from the BBF-WEAP approach are identical to those reported in the URS Corporation (2002a) report (see Table 6), which was expected since the same tissue concentrations and TRV values were used. As stated above, the EHQs obtained by the TBP-WEAP approach (see Table 6) are slightly different from those reported in the Langley RI report (URS Corporation 2002a) due to the fact that the computed tissue residues are different from those measured. The EHQ values obtained by TrophicTrace (see Table 6) are identical to those computed with TBP-WEAP for the organic chemicals as expected. Of course, the EHQ associated with arsenic is quite different from the value reported in the RI report because the computed tissue residue was so different from that measured for arsenic.

**Table 6**  
**EHQs (NOAEL-Based) for Benthic Invertebrates Assessment Endpoint**

Contaminant	EHQ using Known Body Burden (unitless)		EHQs Using Calculated Body Burden	
	Langley RI Report	BBF-WEAP	TBP-WEAP	TrophicTrace
Benzo(a)pyrene	2.28E+01	2.28E+01	2.17E+01	2.17E+01
PCB (Aroclor 1254)	4.18E+02	4.18E+02	3.96E+02	3.96E+02
Arsenic	1.42E+00	1.42E+00	NA *	1.54E-03

\* Not Applicable; See discussion in text.

Figures 6 and 7 show time-series plots of calculated benthic invertebrate tissue concentration and EHQ, respectively, for PCB (Aroclor 1254) using the RECOVERY model as input into TBP and TBP as input into WEAP. These graphs indicate that ARAMS can be used to predict future risks based on the initial conditions. For this site, results indicate that ecological risks would decrease to acceptable levels after about 40 years. Continued loadings could have been assessed as well. These results are time-varying because RECOVERY was used to compute time-varying sediment and water concentrations, those results were passed to TBP to obtain time-varying tissue residues, and those results were used by WEAP to produce time-varying EHQ. These results illustrate the capability to predict future risks with natural recovery or attenuation of contamination.

The BBF-WEAP calculations, the TBP-WEAP calculations, the TrophicTrace, and the Langley RI report all reach the same conclusions: PCB (Aroclor 1254) and benzo(a)pyrene sediment concentrations may pose hazards to benthic invertebrates since the EQHs were greater than 1.0. However, the TrophicTrace results for arsenic suggest that there is no reason for concern, which is not the same conclusion reached in the RI report. The BCF derived estimate of benthic invertebrate arsenic tissue concentration (1.31E-02 mg/kg) was much smaller than the measured value (12.1 mg/kg). This application pointed out the need to add a BCF module within FRAMES to allow estimation of tissue concentrations based on water concentrations. Such a module should be linked to a broad database of BCF values, such as the one that exists in USEPA's ECOTOX Database. These capabilities were being added to ARAMS at the time this report was prepared.

### Atlantic croaker (fish)

ARAMS/FRAMES BBF-WEAP modules and TrophicTrace were used to estimate the risk for Atlantic croaker with a lipid content of 5.42 percent (RI report, URS Corporation 2002a). The diet tissue concentrations and other constant values needed for the calculations for Atlantic croaker are given in Table 7 based on information in the RI report.

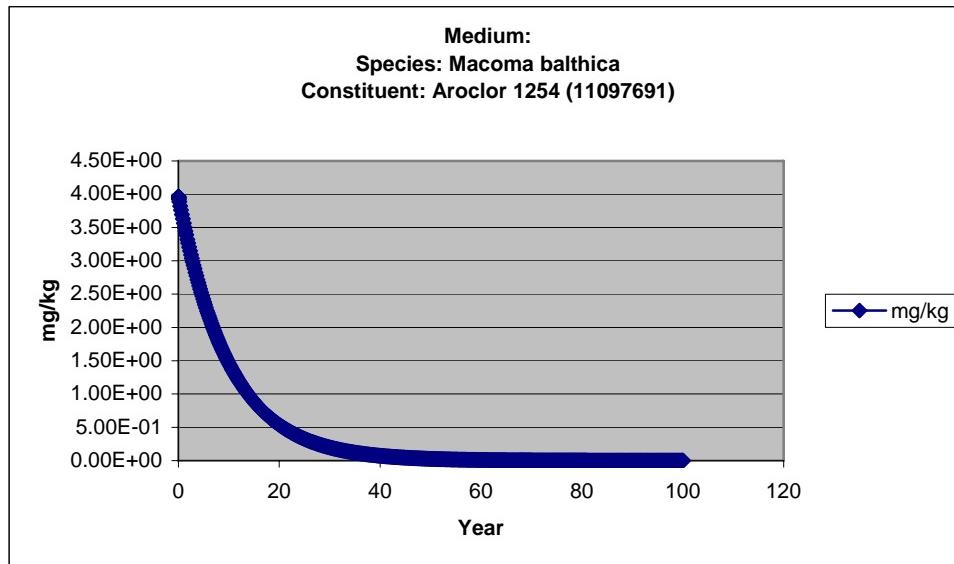


Figure 6. Benthic invertebrate tissue concentration computed by TBP for PCB (Aroclor 1254) using sediment concentrations computed by RECOVERY

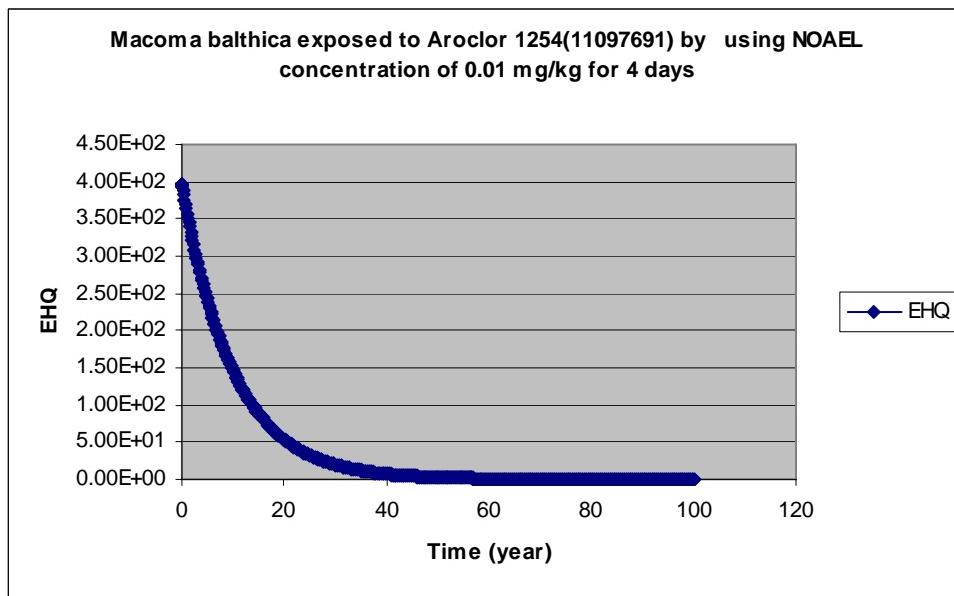


Figure 7. EHQ for benthic invertebrates calculated with WEAP for PCB (Aroclor 1254) using output from TBP

The current TrophicTrace model (version 3.042) is parameterized for the fish species mummichog and summer flounder. In this demonstration, the TrophicTrace parameters of summer flounder were replaced with the parameters for Atlantic croaker (piscivorous fish). The diet of the Atlantic croaker was assumed to consist of 33.3 percent benthic invertebrates, 33.3 percent bivalves, and 33.4 percent killifish (Table 7). TrophicTrace input is provided on the

**Table 7**  
**Atlantic Croaker Diets Used for Screening Assessment of Hazard Quotients**

Constituent of Potential Ecological Concern	Maximum Sediment Concentration (mg/kg)	Maximum Bivalve Concentration (mg/kg)	Maximum Benthic Invertebrate Concentration (mg/kg)	Maximum Small Fish Concentration (mg/kg)
Benzo(a)pyrene	27.4	4.37E-02	27.4	0
PCB (Aroclor 1254)	4.18	3.56E-02	4.18	1.06E-01
Arsenic	12.1	14.3	12.1	1.59E+00
Croaker Constants: Food Ingestion Rate (FI) = 0.054 kg/day Sediment Ingestion Rate (SI) = 0.0081 kg/day Bivalve Ingestion Fraction (Fbiv) = 0.333 unitless Benthic Invertebrate Fraction (Fbin) = 0.333 unitless Body Weight (BW) = 0.23 kg Area Use Factor = 1 unitless Source: Table H1-2 (URS Corporation 2002b)				

enclosed compact disk. TrophicTrace utilizes the Gobas (1993) model (Equation 3) to estimate fish body burdens for hydrophobic organic compounds. Thus, this demonstration used the Gobas (1993) model to estimate Atlantic croaker and killifish PCB and benzo(a)pyrene tissue concentrations. TrophicTrace utilizes TBP (Equation 2) to compute concentrations of nonpolar organic chemicals in tissue of sediment-dwelling organisms. TBP was used to estimate bivalve, benthic invertebrate, killifish, and blue crab PCB and benzo(a)pyrene tissue concentrations. TrophicTrace uses TTF and BCF approaches to estimate fish body burdens for inorganic and hydrophilic compounds (von Stackelberg and Burmistrova 2003). The BCF method was used to estimate the Atlantic croaker, bivalve, benthic invertebrate, killifish and blue crab arsenic tissue concentrations. TrophicTrace uses estimated or user supplied diet tissue concentrations. This demonstration illustrates both methods. TrophicTrace output using estimated diet tissue concentrations is shown in Appendix B. TrophicTrace results for user-supplied diet tissue concentrations are shown in Appendix C.

At the time that this report was prepared, ARAMS/FRAMES did not have a module similar to the Gobas (1993) model to compute fish tissue concentrations, such as the approach in TrophicTrace. However, the FISHRAND model (Menzie-Cura & Associates, Inc. 2003) was being added at that time. FISHRAND uses a dynamic form of the Gobas (1993) model, and was being incorporated into ARAMS/FRAMES so that time-varying water and sediment concentrations could be passed to it, and it would pass time-varying tissue concentrations to WEAP to obtain EHQ values over time.

Using the Gobas (1993) model in TrophicTrace along with the estimated diet tissue concentrations (Appendix B), the estimated PCB (Aroclor 1254) fish tissue concentration ( $C_f$ ) is 7698.48 µg/kg or 7.70 mg/kg (Table 8 and Appendix B). Using user-supplied diet tissue concentrations, the PCB (Aroclor 1254)  $C_f$  is 2.64 mg/kg (Table 8 and “Bioaccumulation in Fish” in Appendix C). Field-collected fish samples include Atlantic croaker, summer flounder, striped bass, and weakfish. The field-collected fillet concentrations (URS Corporation 2002b) ranged from 3.11E-02 to 3.08E-01 mg/kg (Table 8), which is much

**Table 8**  
**Daily Dose and Measured and Estimated Tissue Concentrations for Atlantic Croaker**

Contaminant	Maximum Dose Concentration for Atlantic Croaker (mg/kg BW/day) from Langley RI <sup>1</sup>	Tissue Concentration in Atlantic Croaker (mg/kg wet)		
		Known Tissue Concentration <sup>2</sup>	Estimated Tissue Concentration from TrophicTrace Using Measured Diet Concentrations	Estimated Tissue Concentration from TrophicTrace Using Estimated Diet Concentrations
Benzo(a)pyrene	3.11E+00	ND	1.66E+01 <sup>3</sup>	4.87E+01 <sup>3</sup>
PCB (Aroclor 1254)	4.85E-01	3.11E-02 to 3.08E-01	2.64E+00 <sup>4</sup>	7.7E+00 <sup>4</sup>
Arsenic	1.61E+00	7.42E-01 to 2.56E+00	1.31E-02 <sup>3</sup>	1.31E-02 <sup>3</sup>

Note: ND = Not detected.  
<sup>1</sup> Data from Table H1-2 (URS Corporation 2002b).  
<sup>2</sup> Measured Atlantic croaker tissue concentrations from Table E4-2 (URS Corporation 2002b).  
<sup>3</sup> BCF method used, and diets are not used.  
<sup>4</sup> Gobas (1993) model was used.

smaller than both estimated values. Overestimation of fish tissue residue may be due to the fish parameters used in Gobas (1993) model in TrophicTrace because the measured and predicted food concentrations were of similar magnitude. These fish concentration levels could be impacted by the Atlantic croaker's ability to metabolize and degrade contaminants at a higher rate than predicted by the model.

TRV values based on average daily dose and tissue concentrations are provided in Table 9. Unfortunately, the EHQs reported in the RI report cannot be compared with those computed from ARAMS. Aquatic EHQ in ARAMS is based on tissue residue, whereas the EHQ results in the RI report were based on dose. URS Corporation (2002a) used equations similar to Equations 4 and 5 to estimate the average daily dose for the Atlantic croaker (Table 8).

The EHQ estimates from TrophicTrace and the WEAP module are shown in Table 10. TrophicTrace EHQs shown in Table 10 correspond to the toxicity quotients (TQs) shown in Appendixes B and C (see "Summary for Fish"). Appendix B provides TrophicTrace output using calculated concentrations as input, and Appendix C shows TrophicTrace output using measured concentrations as input. The TrophicTrace used the trapezoidal fuzzy numbers to characterize the Atlantic croaker tissue concentrations. The four numbers used represent the minimum value, the mean, the 95 percent upper confidence limit, and the maximum value.

**Table 9**  
**TRV (NOAEL) Values for Atlantic Croaker**

Contaminant	TRV Based on Dose Concentration (mg/kg BW/day)	Reference	TRVs Based on Tissue Concentration (mg/kg)	Reference
Benzo(a)pyrene	6.30E-05	USEPA (1997)	1.90E+00	PCB (Aroclor 1254) used as surrogate; Hansen et al. (1974)
PCB (Aroclor 1254)	6.30E-07	Virginia Water Quality Criteria (1995)	1.90E+00	Hansen et al. (1974)
Arsenic	4.00E-03	Virginia Water Quality Criteria (1995)	4.70E-01	Dixon and Sprague (1981)

**Table 10**  
**NOAEL-Based EHqs for the Atlantic Croaker Assessment Endpoint**

Contaminant	EHQs Using Dose Concentration Langley RI <sup>1</sup>	EHQs Using Tissue Concentration			
		Known Body Burden (BBF)	Known Body Burden (TrophicTrace)	TrophicTrace Using Measured Diet Concentrations	TrophicTrace Using Estimated Diet Concentrations
Benzo(a)pyrene	4.94E+04	0.00E+00	0.00E+00	8.74E+00	2.56E+01
PCB (Aroclor 1254)	7.70E+05	1.64E-02 -- 1.62E-01	1.64E-02 -- 1.62E-01	1.39E+00	4.05E+00
Arsenic	4.02E+02	1.58E+00 -- 5.45E+00	1.58E+00 -- 5.45E+00	2.79E-02	2.79E-02

<sup>1</sup> RS Corporation (2002a).

The NOAEL-based EHqs for Atlantic croaker exposed to PCB (Aroclor 1254), arsenic, and benzo(a)pyrene reported in the Langley RI report are greater than 1.0 (URS Corporation 2002a). The known BBF-WEAP approach yields the same results for EHQ as TrophicTrace using known Atlantic croaker tissue concentrations (Table 10), which should be the case. The TrophicTrace EHQ results using estimated Atlantic croaker tissue concentrations indicate that the PCB (Aroclor 1254) and benzo(a)pyrene EHqs were greater than 1.0, and the arsenic EHQ was less than 1.0.

TrophicTrace used BCF to estimate arsenic tissue concentrations in Atlantic croaker. The BCF estimate for arsenic resulted in a fish tissue concentration that was much smaller than the measured (i.e., 0.742 – 2.56 mg/kg measured versus 1.31E-02 mg/kg from BCF) as indicated in Table 8. Obviously, much more accurate estimates for BCF values are needed, or an alternative method for estimating tissue residue for inorganic constituents is required.

### Belted kingfisher (avian)

The food chain model (Equation 4) in TrophicTrace was used to estimate total daily oral exposure dosage for the belted kingfisher. The belted kingfisher's diet is composed of 87 percent killifish and 13 percent blue crab. Body weight, ingestion rate, and other parameters are given in Table 11 notes. TrophicTrace used TBP to estimate organic tissue concentrations of organisms in the diet, and BCF to estimate inorganic tissue concentrations of organisms in the diet. The computed diet concentrations are shown in Appendix B (see "Chemical Parameters for Birds").

The recommended TRV values for belted kingfisher (URS Corporation 2002b) are given in Table 12. The RI reported and computed daily dose and EHQ values are given in Table 13. The computed values are from TrophicTrace using measured and estimated diet tissue concentrations. The NOAEL-based EHqs from TrophicTrace using the measured diet concentrations agree with those from the RI report and are less than 1.0 for the belted kingfisher. The TrophicTrace

**Table 11**  
**Belted Kingfisher Measured Diet Tissue Concentrations**

Constituent of Ecological Concern	Maximum Whole Crab Concentration (mg/kg)	Maximum Small Fish Concentration (mg/kg)	Maximum Surface Water Concentration (mg/kg)
Benzo(a)pyrene	ND	ND	ND
PCB (Aroclor 1254)	0.00E+00	1.06E-01	0.00E+00
Arsenic	2.84E+00	1.59E+00	3.74E-03
Kingfisher constants: Food Ingestion Rate (FI) = 0.107 kg/day Water Ingestion Rate (WI) = 0.021 L/day Fish Ingestion Fraction (Ffish) = 0.87 unitless Crab Ingestion Fraction (Fcrab) = 0.13 unitless Body Weight (BW) = 0.125 kg			
Source: Table H1-3 and Appendix C (URS Corporation 2002b)			

**Table 12**  
**NOAEL-Based TRV Values for Belted Kingfisher**

Contaminant	TRV (mg/kgBW/day)	Reference
Benzo(a)pyrene	8.47E-02	Hough et al. (1991)
PCB (Aroclor 1254)	4.40E-01	Opresko et al. (1996)
Arsenic	5.14E+00	Opresko et al. (1996)
Source: Table H1-3 (URS Corporation 2002b).		

**Table 13**  
**Belted Kingfisher Estimated Daily Doses and EHQ (HQ) Based on NOAEL TRV Values for the Belted Kingfisher Assessment Endpoint**

Contaminant	Daily Doses			EHQ (TQ)		
	Langley RI Reported Values <sup>1</sup>	Trophic Trace with Measured Diet Concentrations	Trophic Trace with Estimated Diet Concentrations	Langley RI Reported Values <sup>1</sup>	Trophic Trace with Measured Diet Concentrations	Trophic Trace with Estimated Diet Concentrations
Benzo(a)pyrene	0.00E+00	0.00E+00	2.39E+01	0.00E+00	0.00E+00	2.83E+02
PCB (Aroclor 1254)	7.89E-02	7.89E-02	3.85E+00	1.79E-01	1.79E-01	8.74E+00
Arsenic	1.50E+00	1.50E+00	1.12E-02	2.92E-01	2.92E-01	2.18E-03

<sup>1</sup> Table H1-3 (URS Corporation 2002b).

results using estimated diet tissue concentrations indicated that both organic constituents have an EHQ greater than 1.0 and may cause adverse health effects to the belted kingfisher. TrophicTrace overestimated organic chemical tissue concentrations in killifish and blue crabs (see “Bioaccumulation in Fish” and “Bioaccumulation in Invertebrates,” respectively; Appendix B), resulting in an overly conservative daily dose and EHQ estimate (Table 13). TrophicTrace, using BCF, underestimated arsenic tissue concentrations in killifish and blue

crabs (i.e., killifish value of 1.59 mg/kg measured versus 1.31E-02 mg/kg estimated; blue crab value of 2.84 mg/kg measured versus 1.31E-02 mg/kg estimated) (see “Bioconcentration in Aquatic Species,” Appendix C). Thus, the arsenic BCF value is too small and produces hazard results that are not conservative enough. Benzo(a)pyrene was not detected in diets of belted kingfisher (Table 11), but TropicTrace computed diet concentrations and thus non-zero daily dose and EHQ (Table 13).

### Mink (mammal)

TrophicTrace version 3.042 is parameterized for the mink and the otter mammalian receptors. This demonstration used the same mink body weight, ingestion rate, and diet composition values as the Langley RI report. Table 14 shows the diet information and other parameter values needed for the ERA of mink. This information is also included on the enclosed compact disk. TrophicTrace used a food chain model (Equation 5) to estimate total daily oral exposure dosage for the mink. The daily oral exposure doses are shown in Table 15.

The TRV values (URS Corporation 2002a) for mink are given in Table 16. The Langley RI results and the TrophicTrace results agree as expected when using measured diet tissue concentrations and indicate that the NOAEL-based EHQs for the mink are greater than 1.0 for all three constituents (Table 17 and “Summary for Mammals” in Appendix C). Thus, a risk assessor using TrophicTrace would reach the same conclusions as those found in the Langley RI report: sediment concentrations may pose a significant hazard to mink. The TrophicTrace results when using estimated diet tissue concentrations indicated that Aroclor 1254 and benzo(a)pyrene may cause adverse health effects to mink, but arsenic will not. The EHQs for the organic constituents using computed diet concentrations were remarkably close to those for measured diet concentrations indicating good estimates of diet concentrations. The EHQ for arsenic using computed diet concentrations was substantially less than that for measured diet concentrations, again indicating the need for more accurate methods for estimating tissue concentrations for inorganic constituents.

<b>Table 14</b> <b>Mink Measured Diet Concentrations</b>			
<b>Constituent of Potential Ecological Concern</b>	<b>Maximum Surface Water Concentration (mg/L)</b>	<b>Maximum Small Fish Concentration (mg/kg)</b>	<b>Maximum Benthic Invertebrate Concentration (mg/kg)</b>
Benzo(a)pyrene	0.0E+00	0.0E+00	2.74E+01
PCB (Aroclor 1254)	0.0E+00	1.06E-01	4.18E+00
Arsenic	3.74E-03	1.59E+00	1.21E+01
Mink constants: Food ingestion Rate (FI) = 0.178 kg/day Water Ingestion Rate (WI) = 0.11 L/day Fish Ingestion Fraction (Ffish) = 0.5 unitless Benthic Invertebrate Ingestion Fraction = 0.5 unitless Body Weight (BW) = 0.8 kg Source: Table H1-4 (URS Corporation 2002b)			

**Table 15**  
**Mink Total Daily Oral Exposure Doses**

Contaminant	Exposure Dose (mg /kg BW/day)		
	Langley RI Reported Values	TrophicTrace with Measured Diet Concentrations	TrophicTrace with Estimated Diet Concentrations
Benzo(a)pyrene	3.01E+00	3.01E+00	6.02E+00
PCB (Aroclor 1254)	4.71E-01	4.71E-01	9.47E-01
Arsenic	1.51E+00	1.51E+00	2.88E-03

Note: TrophicTrace calculations used data from Table H1-4 (URS Corporation 2002a).

**Table 16**  
**NOAEL-Based TRV Values for Mink**

Contaminant	TRV (mg/kgBW/day)	Reference
Benzo(a)pyrene	1.00E+00	Opresko et al. 1996
PCB (Aroclor 1254)	1.40E-01	Opresko et al. 1996
Arsenic	1.26E-01	Opresko et al. 1996

**Table 17**  
**EHQ Values for Mink Assessment**

Contaminant	EHQ		
	Langley RI Reported Values	TrophicTrace with Measured Diet Concentrations	TrophicTrace with Estimated Diet Concentrations
Benzo(a)pyrene	1.20E+01	1.20E+01	2.28E-02
PCB (Aroclor 1254)	3.01E+00	3.01E+00	6.02E+00
Arsenic	3.37E+00	3.37E+00	6.76E+00

TrophicTrace overestimated tissue concentrations in killifish (i.e., PCB (Aroclor 1254) value of 1.06E-01 mg/kg measured versus 4.64 mg/kg estimated; benzo(a)pyrene was not detected versus 3.03E+01 mg/kg estimated; see “Bio-accumulation in Fish,” Appendix C) for both organic chemicals. The Gobas (1993) model did not accurately estimate killifish organic tissue concentrations. However, the use of larger values produces conservative hazard results. Trophic-Trace used BCF to estimate killifish and benthic invertebrate tissue concentrations of arsenic. TrophicTrace underestimated arsenic tissue concentrations in killifish and benthic invertebrates (i.e., killifish value of 1.59 mg/kg measured versus 1.31E-02 mg/kg estimated; benthic invertebrates value of 12.1 mg/kg measured versus 1.31E-02 mg/kg estimated) (“Bioconcentration in Aquatic Species,” Appendix C). Thus, the BCF value is too small and produces hazard results that are not conservative enough.

## **Analysis of aquatic demonstration**

The ARAMS application for the Langley site reached the same general hazard conclusions as the Langley RI report (URS Corporation 2002a). ARAMS risks were identical to those reported for the benthic invertebrate, belted king-fisher, and mink when using measured body burdens or diet tissue concentrations (Tables 6, 13, and 17). The Langley RI Report and ARAMS used two different methods to estimate risk for Atlantic croaker, the former being dose based and the later being based on tissue residue. As expected, the risk results based on dose concentration could not be directly compared to the results based on tissue residue (Table 10). The Langley RI results indicate that PCB (Aroclor 1254), arsenic, and benzo(a)pyrene concentrations in sediment may cause adverse health effects to Atlantic croaker (Table 10), whereas mixed results were predicted using the risk approach in ARAMS based on tissue residue.

Computed benthic invertebrate tissue concentrations using BSAF and TBP were in close agreement with measured values. Computed tissue concentrations for fish using the Gobas (1993) model were not as close to measured as desired, indicating a need to improve the parameterization for this model. The BCF value used for arsenic appears to be far too low when comparing measured and computed tissue concentrations. This observation points to the importance of having measured tissue and diet concentrations for inorganics, which ARAMS can accommodate.

## 5 Terrestrial Site

## Pueblo Chemical Depot Site ERA

The site for the ARAMS terrestrial ecological demonstration application is the TNT Washout Facility and Discharge System (identified as SWMU 17) located in the southwestern portion of PCD (Figure 8). From the 1940s to 1974, TNT from various munitions was reclaimed at this site, which has an area of 1.7 acres (Earth Tech 2002, Parsons Engineering Science, Inc. 1999). Operations included high-pressure steam washout, drying, flaking, palletizing, and packaging of TNT. Most of the wastewater was treated by filtering, settling, and allowing the remaining liquid to flow to an outdoor sump. The overflow from the sump was discharged into a quarter-mile-long drainage ditch that drains to an evaporative lagoon.



Figure 8. Pueblo Chemical Depot located in Pueblo County, Colorado

Recent reports provide the results of a SERA and an RCRA facility investigation (Earth Tech 2002, Parsons Engineering Science, Inc. 1999). Hazards to a primary consumer/omnivore (deer mouse), an upper tropic level mammalian predator (swift fox), and two upper trophic level avian predators (ferruginous hawk and western meadowlark) were evaluated (Table 18). The COCs at SWMU 17 include TNT, 2,4-dinitrotoluene, 2,6-dinitrotoluene, HMX, and 1,3,5-TNB.

**Table 18**  
**Terrestrial Receptor Species Chosen to Represent Assessment Endpoints for the Pueblo Chemical Depot**

Terrestrial Receptor Functional Groups	Endpoint Species by Community			
	Shortage Prairie	Northern Sandhill Prairie	Greasewood Scrub	Riparian Woodland
Mammal	Primary Consumer/Omnivore			
	Deer mouse	Deer mouse	Deer mouse	Deer mouse
Bird	Higher Level Consumer/Predator			
	Western meadowlark	Western meadowlark	Western meadowlark	Western meadowlark
Mammal	Ferruginous hawk	Ferruginous hawk	Ferruginous hawk	Ferruginous hawk
	Swift fox	Swift fox	Swift fox	Swift fox
Adapted from Table 5.2 of Earth Tech (2002).				

Exposure pathways considered in the original risk assessment include ingestion and dermal contact of surface and subsurface soil and food ingestion via uptake of contaminants by plants from the surface soil. Inhalation of contaminants from subsurface soil was a potential exposure pathway for burrowing animals; however, inhalation pathways were not evaluated due to their minimal contribution to the total exposure dose when compared to ingestion pathways. Storm water runoff may also result in exposure through aquatic pathways. The exposure pathways for terrestrial mammals can be depicted as: soil  $\Rightarrow$  plant  $\Rightarrow$  mammal; soil  $\Rightarrow$  invertebrate  $\Rightarrow$  mammal; and incidental soil ingestion  $\Rightarrow$  mammal. The exposure pathways for birds are: soil  $\Rightarrow$  plant  $\Rightarrow$  mammal; soil  $\Rightarrow$  invertebrate  $\Rightarrow$  mammal; mammal  $\Rightarrow$  bird; and incidental soil ingestion  $\Rightarrow$  bird.

Two different soil depth intervals (0 to 2 ft, surface soil; and 0 to 12.5 ft, subsurface soil) were used for the data collection and EHQ calculations as described in the site ERA report (Earth Tech 2002, Parsons Engineering Science, Inc. 1999). For each soil sample location, the core of soil over the depth interval was mixed and analyzed for chemical concentrations. Borings were taken at multiple locations around the site. The maximum concentration is the maximum concentration that was detected for each of the soil depth intervals. For this ARAMS demonstration, results from both the 0- to 2- and the 0- to 12-ft sampling depth were used.

For this demonstration, the following exposure pathways to the ecological receptors were prescribed through the ingestion route:

- Ingestion of soil or sediment.
- Ingestion of aquatic and terrestrial vegetation.
- Ingestion of aquatic and terrestrial prey items.
- Ingestion of surface water.

The comprehensive ERA process at PCD consisted of three tiers (Earth Tech 2002, Parsons Engineering Science 1999):

- Tier 1 – Evaluation of Detection Limits and Background Concentrations.
- Tier 2 (A, B, and C) – Preliminary Risk Evaluation (PRE).
- Tier 3 – Focused Baseline ERA.

From the above listed tiers, only the first two tiers (SERA) were reported and available for this demonstration. A brief description of Tier 2 (A, B, and C) of the ERA process is provided herein. The ARAMS application was conducted only for Tier 2C due to the limited scope of this demonstration application and because this tier option provides information that can be readily compared with ARAMS results. It should also be noted that surface water and sediment data from water bodies on the site were not available (collected) for the SERA and this demonstration.

### **Oral exposure dose calculations**

Oral exposure dose (ED) is based on ingestion of food and water and incidental ingestion of media (e.g., soil) and requires estimates of diet concentrations. The uptakes in soil invertebrates were estimated using chemical-specific BAFs (bioaccumulation factors) and measured soil concentration, and the uptake in plants was estimated using BCFs (bioconcentration factors) and measured soil concentrations (Earth Tech 2002, Parsons Engineering Science 1999). BAFs and BCFs were derived using regression equations (Earth Tech 2002, Parsons Engineering Science 1999) based on chemical-specific  $K_{ow}$  values (Table 19), hence, contributing to the uncertainty for these exposure concentrations used in risk calculations. In accordance with current USEPA guidance (USEPA 1997), a SERA assumes that a receptor intake is based on 100 percent bioavailability and the most sensitive life stage. These assumptions when combined are likely to overestimate ecological risk. Other required parameters used to calculate ED are given in Table 20.

### **Risk estimations**

In Tiers 2A and 2B, as described in the ERA report (Earth Tech 2002), EHQ was calculated by dividing exposure point concentration (i.e., the maximum concentration) by the respective benchmark value (i.e., soil screening level, or SSL) as a method of evaluating the potential risks posed by contaminants to the receptors representing the assessment endpoints in the study area.

**Table 19**  
**BCF and BAF Parameters Used to Calculate Diet Concentrations for Oral Exposure Dose**

Constituent	CAS Number	Octanol-Water Partition Coefficient		Tier 2C				
		Log $K_{ow}$	$K_{ow}$	$BCF_{sp}^1$	$BCF_{sp}^2$	$BAF_{si}^3$	$BAF_{pm}^4$	$BAF_{im}^5$
2,4-Dinitrotoluene	121-14-2	1.98E+00	9.55E+01	2.40E+00	2.48E+00	5.59E-01	1.63E-05	1.63E-05
2,6-Dinitrotoluene	606-20-2	1.72E+00	5.25E+01	3.3E+00	3.51E+00	5.42E-01	8.81E-06	8.81E-06
Octahydro-1,3,5,7-tetrazocine (HMX)	2691-41-0	6.00E-01	3.98E+00	1.51E+01	1.56E+01	4.77E-01	6.14E-07	6.14E-07
1,3,5-Trinitrobenzene	99-35-4	1.18E+00	1.51E+01	6.96E+00	7.19E+00	5.10E-01	2.44E-06	2.44E-06
2,4,6-Trinitrotoluene	118-96-7	2.25E+00	1.78E+02	1.68E+00	1.73E+00	5.77E-01	3.11E-05	3.11E-05

Note: All BCFs and BAFs are wet-weight basis. Source: Earth Tech (2002), Parsons Engineering Science (1999)

<sup>1</sup> Bioconcentration factor, soil-to-plant (mg/kg plant)/(mg/kg soil), used for deer mouse, swift fox, and ferruginous hawk exposure dose calculations.

<sup>2</sup> Bioconcentration factor, soil-to-plant (mg/kg plant)/(mg/kg soil), used for the western meadowlark exposure dose calculations.

<sup>3</sup> Bioaccumulation factor, soil-to-invertebrate (mg/kg invertebrate / mg/kg soil).

<sup>4</sup> Bioaccumulation factor, plant-to-mammal (mg/kg mammal)/(mg/kg plant).

<sup>5</sup> Bioaccumulation factor, invertebrate-to-mammal (mg/kg mammal)/(mg/kg invertebrate).

**Table 20**  
**Tier 2C Exposure Factors for Pueblo Chemical Depot**

Receptor	Body Weight (g)	Food Ingestion Rate (wet wt basis) (g/g-day)	Water Ingestion Rate (ml/g-day)	Incidental Soil Ingestion Rate (% of diet)	Home Range (acres)	Dietary Composition
Swift fox	2,250 USEPA (1993): Midpoint of range for the species	0.088 Sample et al. (1997): Mean for the kit fox	0.020 Sample et al. (1997): Minimal, may obtain all needed water from prey	4 Estimated based on data for red fox in Beyer et al. (1994) and USEPA (1993)	1,140 Sample et al. (1997): Mean for kit fox in California and western Arizona	100 percent small mammals Sample et al. (1997)
Deer mouse	21 USEPA (1993): Mean of North American body weights (adult females & males)	0.200 USEPA (1993): Mean value for nonlactating adults	0.190 USEPA (1993): Mean value for adults (male & female)	2 Estimated based on data for white footed mouse in Beyer et al. (1994) and USEPA (1993)	0.06 USEPA (1993): Mean for males & females in Utah (summer & winter)	40 percent arthropods, 60 percent plants USEPA (1993): approx of findings from study in short grass prairie in Colorado
Ferruginous hawk	1,145 Dunning (1993): Mean of adult male & female body weights	0.100 USEPA (1993): Mean of summer and winter values for red-tailed hawk	0.057 USEPA (1993): Mean of male and female values for red-tailed hawk	2 Estimated based on data for other species in Beyer et al. (1994) and USEPA (1993)	5,000 USEPA (1993): Estimate based on mean for red-tailed hawk in Colorado upland prairie	100 percent small mammals USEPA (1993): based on red-tailed hawk
Western meadowlark	104.6 Sample et al. (1997): Average of male & female body weights	0.043 Calculated based on data in Sample et al. (1997)	0.190 Pierce (1974) in Sample et al. (1997)	2 Estimated based on data for other species in Beyer et al. (1994) and USEPA (1993)	17 Schaeff & Picman (1988) in Sample et al. (1997): Mean territory size Manitoba	63 percent invertebrates 37 percent seeds, Lanyon (1994) in Sample et al. (1997): Based on 1920 samples throughout western North America

Source: Table 5.13 of Earth Tech (2002).

$$EHQ = \frac{\text{Exposure Soil Concentration}}{\text{Benchmark Concentration}} \quad (9)$$

As an example of the use of Equation 9, for TNT and deer mouse, the EHQ in Tier 2A and 2B is calculated as  $EHQ = 3.7E+02/5.75 = 6.4E+01$ . An EHQ value equal to or greater than 1.0 is considered the threshold level at which ecological effects may occur (i.e., the chemical will be retained as a COPEC). An EHQ less than 1.0 indicates that the chemical alone is unlikely to cause adverse ecological effects. For each chemical and species, two values for EHQ were calculated. One EHQ is based on the maximum concentration in soil ( $C_{max}$ ) and another EHQ is based on a 95th percentile upper confidence level (UCL95) concentration ( $C_{95}$ ) as explained below. The  $C_{95}$  soil concentration is lower than the maximum concentration, and therefore produces a lower EHQ value.

The following formula was used in the reported ERA to quantify the UCL95 on the arithmetic mean concentration for log-normal distributed data (USEPA 1992):

$$UCL95 = e^{\left( \bar{x} + 0.5 s^2 + \frac{sH}{\sqrt{n-1}} \right)} \quad (10)$$

where

$e$  = base of natural log, approximately 2.718

$\bar{x}$  = arithmetic mean of the natural logarithms of the analyte concentrations

$s$  = standard deviation of the natural logarithms of the analyte concentrations

$H$  = H-statistics (Gilbert 1987, taken from Land 1975)

$n$  = number of samples

In Tier 2C, EHQs were calculated by dividing the total exposure dose by NOAEL- or LOAEL-based TRVs,

$$EHQ = \frac{\text{Exposure Dose}}{\text{NOAEL or LOAEL}} \quad (11)$$

Again, an EHQ value equal to or greater than 1.0 is considered the threshold level at which ecological effects may occur (i.e., the chemical will be retained as a COPEC), and an EHQ less than 1.0 indicates that the chemical alone is unlikely to cause adverse ecological effects.

### Adjusted NOAEL

The NOAEL based on the test species was adjusted for the body weight of the wildlife species being evaluated, as shown in the following equation modified from Sample et al. (1996). The following equation is used for mammals only; body weight scaling is not conducted for avian species.

$$NOAEL_w = NOAEL_t (bw_t / bw_w)^{1/4} \quad (12)$$

where

$NOAEL_w$  = NOAEL adjusted for wildlife species, mg contaminant/kg body weight/day

$NOAEL_t$  = NOAEL for the test species, mg contaminant /kg body weight/day

$bw_t$  = body weight of the test species, kg

$bw_w$  = body weight for the wildlife species, kg

The adjusted NOAEL values were used for calculation of EHQ for the Tier 2C assessment.

## ARAMS Application

The input data for ARAMS were obtained from Earth Tech (2002) and Parsons Engineering Science, Inc. (1999) reports. The TWEM model in ARAMS was used to estimate the mammal and bird oral exposure doses. The calculated EHQ values from the WEAP module in ARAMS were compared against the reported values. For some of the assessment endpoints, such as western meadow-lark, EHQ was not calculated because no TRV value was available either from the ERA site report or TTD module in ARAMS. The BAF values used in TWEM were calculated from the site BCF and BAF data (Table 19) and other parameters as shown in Table 21.

### Development of conceptual site model (CSM)

The possible exposure routes described in the ERA reports (Earth Tech 2002, Parsons Engineering Science 1999) are shown in Figure 9. However, the CSM that was actually used in the ERA, and for ARAMS, is a simplified version of the original one as shown in Figure 10. The CSM includes primary and secondary sources (i.e., soil and storm water runoff) of contaminants. However, there were no concentrations reported for sediment and water. The risks that were quantified in the ERA assumed that the soil is the source of contamination, and the exposure occurs through ingestion of food and soil. The risks associated with inhalation and dermal contacts were not quantified in the ERA.

Figure 11 shows the ARAMS/FAMES CSM framework that was used for PCD application. Measured concentrations in soil and water could be input via the User Defined Object using the Known SCF and Known WCF modules, respectively. However, as noted above, the water concentrations were zero. TWEM was used to compute ED, and WEAP was used to compute EHQ using TRVs from TTD DCE.

**Table 21**  
**Site Data Used to Calculate BAFs Required for TWEM**

Species	Chemical	0- to 2-ft Soil Sample							Data for TWEM	
		<i>BCF<sub>sp</sub></i> <sup>1</sup>	<i>BAF<sub>pm</sub></i> <sup>2</sup>	<i>BAF<sub>si</sub></i> <sup>3</sup>	<i>BAF<sub>im</sub></i> <sup>4</sup>	<i>F<sub>pm</sub></i> <sup>5</sup>	<i>F<sub>im</sub></i> <sup>6</sup>	<i>BAF<sub>1</sub></i> <sup>7</sup>	<i>BAF<sub>2</sub></i> <sup>7</sup>	
Deer Mouse	2,4-Dinitrotoluene	2.40E+00		5.59E-01				2.40E+00	5.59E-01	
Ferruginous Hawk	2,4-Dinitrotoluene	2.40E+00	1.63E-05	5.59E-01	1.63E-05	0.6	0.4	2.35E-05	3.64E-06	
Western Meadowlark	2,4-Dinitrotoluene	2.48E+00		5.59E-01				2.48E+00	5.59E-01	
Swift Fox	2,4-Dinitrotoluene	2.40E+00	1.63E-05	5.59E-01	2.04E-06	0.6	0.4	2.35E-05	4.56E-07	
Deer Mouse	2,6-Dinitrotoluene	3.39E+00		5.42E-01				3.39E+00	5.42E-01	
Ferruginous Hawk	2,6-Dinitrotoluene	3.39E+00	8.81E-06	5.42E-01	8.81E-06	0.6	0.4	1.79E-05	1.91E-06	
Western Meadowlark	2,6-Dinitrotoluene	3.51E+00		5.42E-01				3.51E+00	5.42E-01	
Swift Fox	2,6-Dinitrotoluene	3.39E+00	8.81E-06	5.42E-01	8.81E-06	0.6	0.4	1.79E-05	1.91E-06	
Deer Mouse	HMX	1.51E+01		4.77E-01				1.51E+01	4.77E-01	
Ferruginous Hawk	HMX	1.51E+01	6.14E-07	4.77E-01	6.14E-07	0.6	0.4	5.56E-06	1.17E-07	
Western Meadowlark	HMX	1.56E+01		4.77E-01				1.56E+01	4.77E-01	
Swift Fox	HMX	1.51E+01	6.14E-07	4.77E-01	7.67E-08	0.6	0.4	5.56E-06	1.46E-08	
Deer Mouse	1,3,5-Trinitrobenzene	6.96E+00		5.10E-01				6.96E+00	5.10E-01	
Ferruginous Hawk	1,3,5-Trinitrobenzene	6.96E+00	2.44E-06	5.10E-01	2.44E-06	0.6	0.4	1.02E-05	4.98E-07	
Western Meadowlark	1,3,5-Trinitrobenzene	7.19E+00		5.10E-01				7.19E+00	5.10E-01	
Swift Fox	1,3,5-Trinitrobenzene	6.96E+00	2.44E-06	5.10E-01	3.05E-07	0.6	0.4	1.02E-05	6.22E-08	
Deer Mouse	2,4,6-Trinitrotoluene	1.68E+00		5.77E-01				1.68E+00	5.77E-01	
Ferruginous Hawk	2,4,6-Trinitrotoluene	1.68E+00	3.11E-05	5.77E-01	3.11E-05	0.6	0.4	3.13E-05	7.18E-06	
Western Meadowlark	2,4,6-Trinitrotoluene	1.73E+00		5.77E-01				1.73E+00	5.77E-01	
Swift Fox	2,4,6-Trinitrotoluene	1.68E+00	3.11E-05	5.77E-01	3.88E-06	0.6	0.4	3.13E-05	8.96E-07	

(Continued)

<sup>1</sup> Bioconcentration factor, soil-to-plant (mg/kg plant)/(mg/kg soil), used for deer mouse, swift fox, and ferruginous hawk exposure dose calculations.<sup>2</sup> Bioaccumulation factor, plant-to-mammal (mg/kg mammal)/(mg/kg plant).<sup>3</sup> Bioconcentration factor, soil-to-plant (mg/kg plant)/(mg/kg soil), used for the western meadowlark exposure dose calculations.<sup>4</sup> Bioaccumulation factor, invertebrate-to-mammal (mg/kg mammal)/(mg/kg invertebrate).<sup>5</sup> *F<sub>pm</sub>* = fraction of plants in diet of the mammal (unitless).<sup>6</sup> *F<sub>im</sub>* = fraction of invertebrates in diet of the mammal (unitless).<sup>7</sup> BAF (1 or 2) = bioaccumulation factor or bioconcentration factor (1 = Biota 1; 2 = Biota 2).

**Table 21 (Concluded)**

Species	Chemical	0- to 12.5-ft Soil Sample							Data for TWEM	
		Site Data								
		<i>BCF</i> <sub>sp</sub> <sup>1</sup>	<i>BAF</i> <sub>pm</sub> <sup>2</sup>	<i>BAF</i> <sub>si</sub> <sup>3</sup>	<i>BAF</i> <sub>im</sub> <sup>4</sup>	<i>F</i> <sub>pm</sub> <sup>5</sup>	<i>F</i> <sub>im</sub> <sup>6</sup>	<i>BAF</i> <sub>1</sub> <sup>7</sup>	<i>BAF</i> <sub>2</sub> <sup>7</sup>	
Deer Mouse	2,4-Dinitrotoluene	2.40E+00		5.59E-01					2.40E+00	5.59E-01
Ferruginous Hawk	2,4-Dinitrotoluene	2.40E+00	1.63E-05	5.59E-01	1.63E-05	0.6	0.4	2.35E-05	3.64E-06	
Western Meadowlark	2,4-Dinitrotoluene	2.48E+00		5.59E-01				2.48E+00	5.59E-01	
Swift Fox	2,4-Dinitrotoluene	2.40E+00	1.63E-05	5.59E-01	1.63E-05	0.6	0.4	2.35E-05	3.64E-06	
Deer Mouse	2,6-Dinitrotoluene	3.39E+00		5.42E-01				3.39E+00	5.42E-01	
Ferruginous Hawk	2,6-Dinitrotoluene	3.39E+00	8.81E-06	5.42E-01	8.81E-06	0.6	0.4	1.79E-05	1.91E-06	
Western Meadowlark	2,6-Dinitrotoluene	3.51E+00		5.42E-01				3.51E+00	5.42E-01	
Swift Fox	2,6-Dinitrotoluene	3.39E+00	8.81E-06	5.42E-01	8.81E-06	0.6	0.4	1.79E-05	1.91E-06	
Deer Mouse	HMX	1.51E+01		4.77E-01				1.51E+01	4.77E-01	
Ferruginous Hawk	HMX	1.51E+01	6.14E-07	4.77E-01	6.14E-07	0.6	0.4	5.56E-06	1.17E-07	
Western Meadowlark	HMX	1.56E+01		4.77E-01				1.56E+01	4.77E-01	
Swift Fox	HMX	1.51E+01	6.14E-07	4.77E-01	6.14E-07	0.6	0.4	5.56E-06	1.17E-07	
Deer Mouse	1,3,5-Trinitrobenzene	6.96E+00		5.10E-01				6.96E+00	5.10E-01	
Ferruginous Hawk	1,3,5-Trinitrobenzene	6.96E+00	2.44E-06	5.10E-01	2.44E-06	0.6	0.4	1.02E-05	4.98E-07	
Western Meadowlark	1,3,5-Trinitrobenzene	7.19E+00		5.10E-01				7.19E+00	5.10E-01	
Swift Fox	1,3,5-Trinitrobenzene	6.96E+00	2.44E-06	5.10E-01	2.44E-06	0.6	0.4	1.02E-05	4.98E-07	
Deer Mouse	2,4,6-Trinitrotoluene	1.68E+00		5.77E-01				1.68E+00	5.77E-01	
Ferruginous Hawk	2,4,6-Trinitrotoluene	1.68E+00	3.11E-05	5.77E-01	3.11E-05	0.6	0.4	3.13E-05	7.18E-06	
Western Meadowlark	2,4,6-Trinitrotoluene	1.73E+00		5.77E-01				1.73E+00	5.77E-01	
Swift Fox	2,4,6-Trinitrotoluene	1.68E+00	3.11E-05	5.77E-01	3.11E-05	0.6	0.4	3.13E-05	7.18E-06	

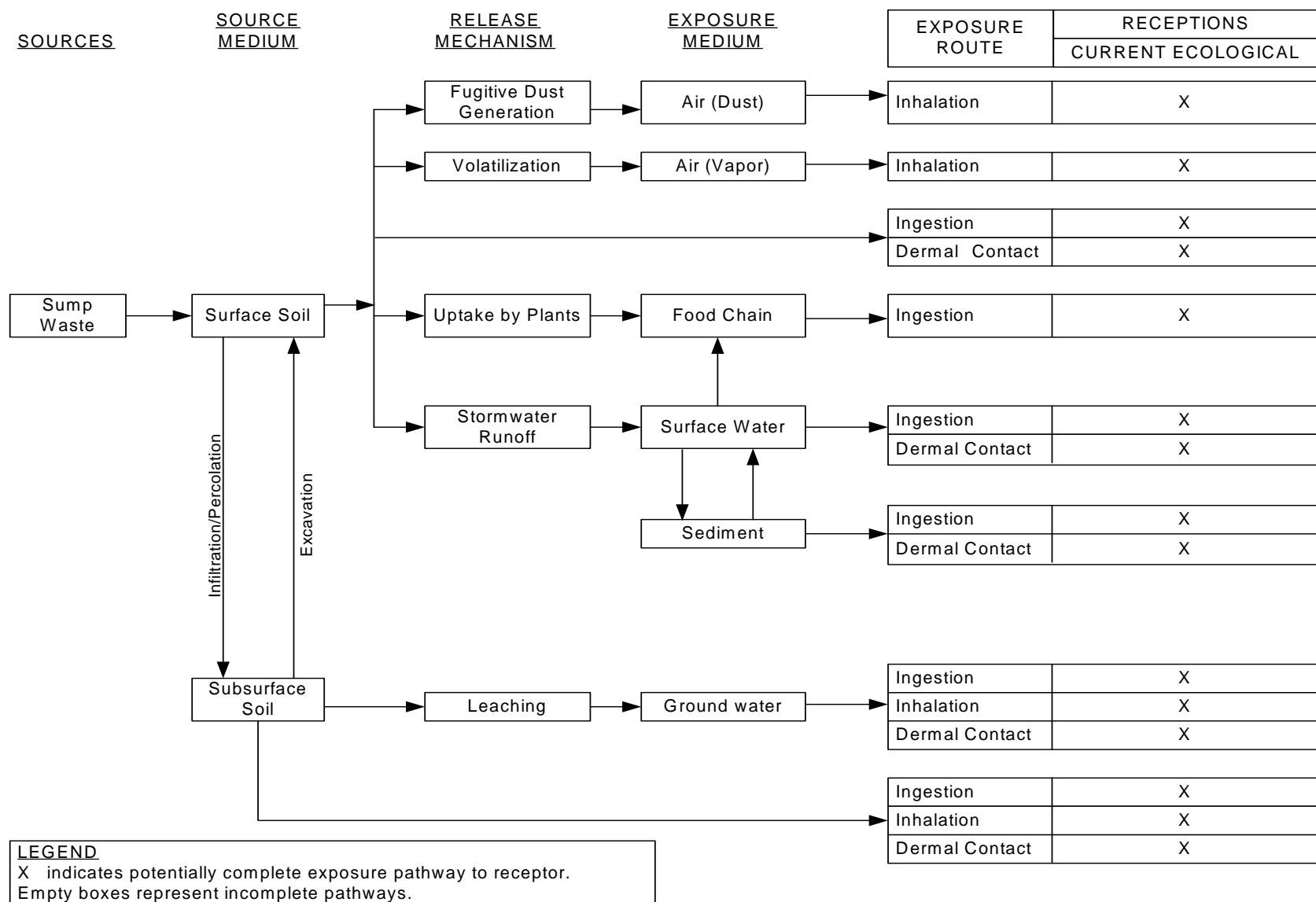


Figure 9. Possible ecological risk assessment conceptual site model for Pueblo site (Earth Tech 2002, Parsons Engineering Science, Inc. 1999)

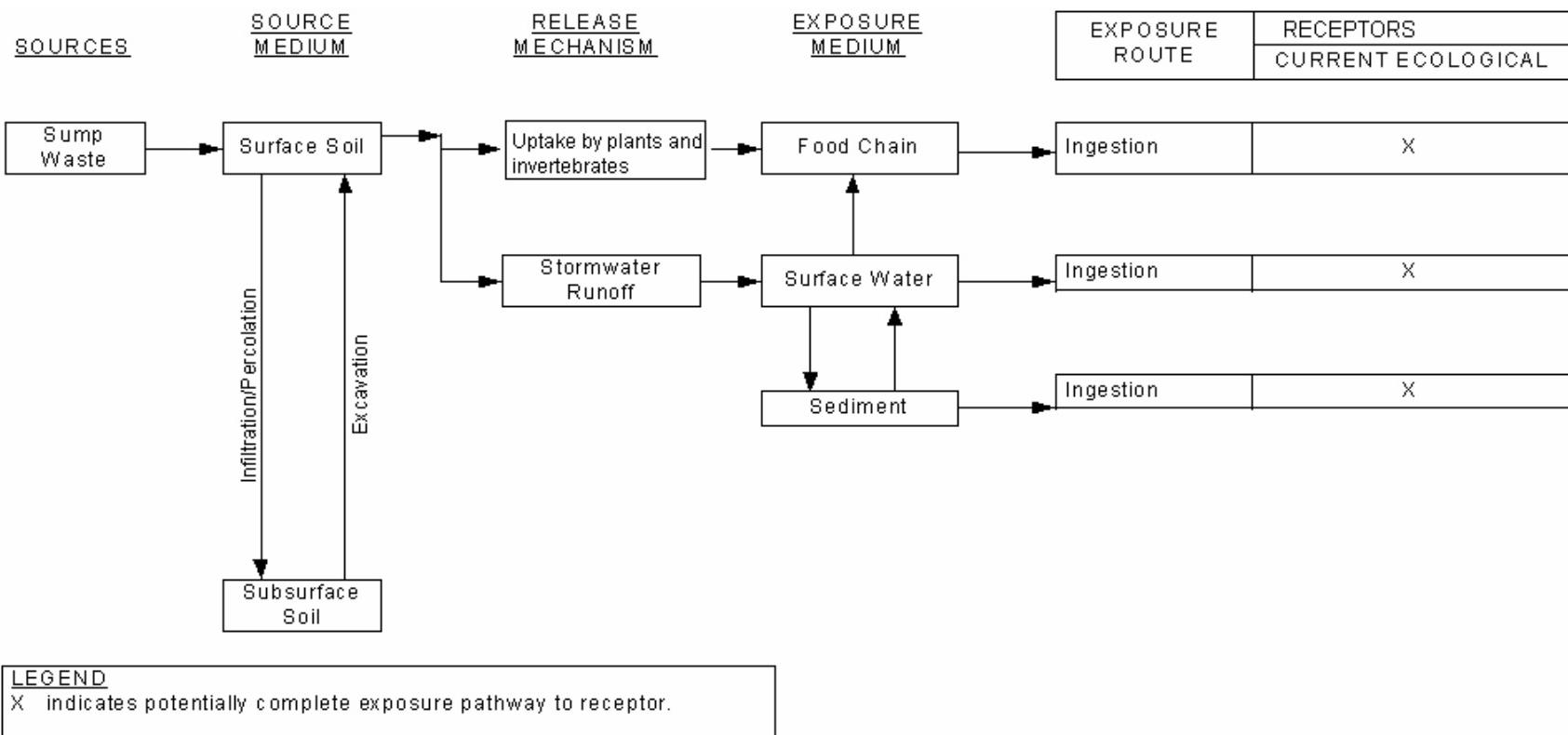


Figure 10. Actual ecological risk assessment conceptual site model used in the ERA and in ARAMS for Pueblo site



Figure 11. ARAMS/FRAMES conceptual site model framework for Pueblo ecological risk assessment

## ED and EHQ Calculations

TWEM uses BAF to calculate food concentrations, whereas some of the values in Table 19 are shown as BCF, which was a term adopted in the ERA report for uptake by plants from soil. The BCF and BAF values in Table 19 are used to calculate values for Known BAF option in TWEM, which are shown in Tables 21 and 22. In some cases, such as the swift fox, it was necessary to multiply BCF and BAF values from the site ERA report to obtain BAF for the diet item in the TWEM.  $BAF_1$  and  $BAF_2$  in Table 21 for ferruginous hawk and swift fox are calculated from the following formulations.

$$\begin{aligned} BAF_1 &= BCF_{sp} \times BAF_{pm} \times F_{pm} \\ BAF_2 &= BAF_{si} \times BAF_{im} \times F_{im} \end{aligned} \quad (13)$$

The EDs were calculated with TWEM, and EHQs were calculated using calculated EDs, appropriate TRVs (NOAEL), and the WEAP module. The reported and calculated ED and EHQ values are provided in Table 23. In Table 22, animal species are numbered from 1 to 4 (1 = deer mouse; 2 = ferruginous hawk; 3 = western meadowlark; 4 = swift fox), and chemicals are numbered from 1 to 5 (1 = 2,4-dinitrotoluene; 2 = 2,6-dinitrotoluene; 3 = HMX; 4 = 1,3,5-trinitrobenzene; 5 = 2,4,6-trinitrotoluene). For some species (actually animal class since TTD searches TRVs based on animal class, e.g., mammalian, avian, etc.) and chemicals, TRVs were not available as indicated by NA in Table 23. For each chemical and species, two EHQs based on maximum concentration and UCL95 concentration were calculated. Additionally, soil concentrations at two depths intervals, 0- to 2-ft and 0- to 12.5-ft intervals, were used in the assessment. EHQ values higher than 1.0 are indicated in red in Table 23.

The TWEM calculated ED and EHQ values equal those reported in the ERA report for the deer mouse, which is expected since the same parameter inputs and TRVs were used. Therefore, the deer mouse verified the dose calculations of TWEM. Calculated ED results for the meadowlark were close to those reported, with the differences due to the fact that the current version of TWEM accepts only integer values for site area, so an area of 2 acres had to be used rather than 1.7 acres as reported. The calculated and reported ED values (and EHQs) for the hawk and fox are slightly different from those reported, due to an input limitation of TWEM. At the time of this study, TWEM would not accept BAF inputs less than 0.001. As can be seen in Table 22, the BAF values for these two receptors are less than 0.001. However, the BAF values had far less contribution to the daily dose rates compared to the contribution from the soil ingestion rates. As a result, the calculated dose for the hawk and fox still were close to the reported values. The differences between the calculated and reported values are due to the site area as mentioned above. After the BAF format limitation in TWEM was discovered through this application, TWEM was modified to remove the input limitation on BAF.

**Table 22**  
**Input Parameters Used in TWEM ED Calculations**

Species	Chemical	0- to 2-ft Soil Sample Concentration									
		BAF <sub>1</sub>	BAF <sub>2</sub>	PBAF1	PBAF2	Cs <sub>95</sub>	Cs <sub>max</sub>	AUF	PS	FIR	NOAEL
1	1	2.40E+00	5.59E-01	0.6	0.38	1.59E-01	1.25	1.00E+00	0.02	0.2	7.88E+00
2	1	2.35E-05	3.64E-06	0	0.98	1.59E-01	1.25	3.40E-04	0.02	0.1	NA
3	1	2.48E+00	5.59E-01	0.62	0.36	1.59E-01	1.25	1.00E-01	0.02	0.043	NA
4	1	2.35E-05	4.56E-07	0	0.96	1.59E-01	1.25	1.49E-03	0.04	0.088	2.45E+00
1	2	3.39E+00	5.42E-01	0.6	0.38	0.00E+00	0	1.00E+00	0.02	0.2	7.88E+00
2	2	1.79E-05	1.91E-06	0	0.98	0.00E+00	0	3.40E-04	0.02	0.1	NA
3	2	3.51E+00	5.42E-01	0.62	0.36	0.00E+00	0	1.00E-01	0.02	0.043	NA
4	2	1.79E-05	1.91E-06	0	0.96	0.00E+00	0	1.49E-03	0.04	0.088	2.45E+00
1	3	1.51E+01	4.77E-01	0.6	0.38	1.50E+00	11	1.00E+00	0.02	0.2	3.28E+00
2	3	5.68E-06	1.17E-07	0	0.98	1.50E+00	11	3.40E-04	0.02	0.1	NA
3	3	1.56E+01	4.77E-01	0.62	0.36	1.50E+00	11	1.00E-01	0.02	0.043	NA
4	3	5.56E-06	1.46E-08	0	0.96	1.50E+00	11	1.49E-03	0.04	0.088	1.02E+00
1	4	6.96E+00	5.10E-01	0.6	0.38	3.97E-01	9.3	1.00E+00	0.02	0.2	7.60E-01
2	4	1.02E-05	4.98E-07	0	0.98	3.97E-01	9.3	3.40E-04	0.02	0.1	NA
3	4	7.19E+00	5.10E-01	0.62	0.36	3.97E-01	9.3	1.00E-01	0.02	0.043	NA
4	4	1.02E-05	6.22E-08	0	0.96	3.97E-01	9.3	1.49E-03	0.04	0.088	2.36E-01
1	5	1.68E+00	5.77E-01	0.6	0.38	5.59E+00	170	1.00E+00	0.02	0.2	9.07E-01
2	5	3.13E-05	7.18E-06	0	0.98	5.59E+00	170	3.40E-04	0.02	0.1	NA
3	5	1.73E+00	5.77E-01	0.62	0.36	5.59E+00	170	1.00E-01	0.02	0.043	NA
4	5	3.13E-05	8.96E-07	0	0.96	5.59E+00	170	1.49E-03	0.04	0.088	2.82E-01
Species	Chemical	0- to 12.5-ft Soil Sample Concentration									
		BAF <sub>1</sub>	BAF <sub>2</sub>	PBAF1	PBAF2	Cs <sub>95</sub>	Cs <sub>max</sub>	AUF	PS	FIR	NOAEL
1	1	2.40E+00	5.59E-01	0.6	0.38	4.37E-01	22	1.00E+00	0.02	0.2	7.88E+00
2	1	2.71E-05	3.64E-06	0.98	0	4.37E-01	22	3.40E-04	0.02	0.1	NA
3	1	2.48E+00	5.59E-01	0.62	0.36	4.37E-01	22	1.00E-01	0.02	0.043	NA
4	1	2.35E-05	3.64E-06	0	0.96	4.37E-01	22	1.49E-03	0.04	0.088	2.45E+00
1	2	3.39E+00	5.42E-01	0.6	0.38	2.08E-01	6.5	1.00E+00	0.02	0.2	7.88E+00
2	2	1.79E-05	1.91E-06	0	0.98	2.08E-01	6.5	3.40E-04	0.02	0.1	NA
3	2	3.51E+00	5.42E-01	0.62	0.36	2.08E-01	6.5	1.00E-01	0.02	0.043	NA
4	2	1.79E-05	1.91E-06	0	0.96	2.08E-01	6.5	1.49E-03	0.04	0.088	2.45E+00
1	3	1.51E+01	4.77E-01	0.6	0.38	1.82E+00	55	1.00E+00	0.02	0.2	3.28E+00
2	3	5.56E-06	1.17E-07	0	0.98	1.82E+00	55	3.40E-04	0.02	0.1	NA
3	3	1.56E+01	4.77E-01	0.62	0.36	1.82E+00	55	1.00E-01	0.02	0.043	NA
4	3	5.56E-06	1.17E-07	0	0.96	1.82E+00	55	1.49E-03	0.04	0.088	1.02E+00
1	4	6.96E+00	5.10E-01	0.6	0.38	1.12E+01	120	1.00E+00	0.02	0.2	7.60E-01
2	4	1.02E-05	4.98E-07	0	0.98	1.12E+01	120	3.40E-04	0.02	0.1	NA
3	4	7.19E+00	5.10E-01	0.62	0.36	1.12E+01	120	1.00E-01	0.02	0.043	NA
4	4	1.02E-05	4.98E-07	0	0.96	1.12E+01	120	1.49E-03	0.04	0.088	2.36E-01
1	5	1.68E+00	5.77E-01	0.6	0.38	4.76E+00	370	1.00E+00	0.02	0.2	9.07E-01
2	5	3.13E-05	7.18E-06	0	0.98	4.76E+00	370	3.40E-04	0.02	0.1	NA
3	5	1.73E+00	5.77E-01	0.62	0.36	4.76E+00	370	1.00E-01	0.02	0.043	NA
4	5	3.13E-05	7.18E-06	0	0.96	4.76E+00	370	1.49E-03	0.04	0.088	2.82E-01

Note: Species: 1 = deer mouse; 2 = ferruginous hawk; 3 = western meadowlark; 4 = swift fox; Chemical: 1 = 2,4-dinitrotoluene; 2 = 2,6-dinitrotoluene; 3 = HMX; 4 = 1,3,5-trinitrobenzene; 5 = 2,4,6-trinitrotoluene; BAF (1 or 2) = bioaccumulation factor or bioconcentration factor (1 = Biota 1; 2 = Biota 2); for more information about the biota (diet type) see Table 20; PBAF (1 or 2) = fraction for diet item 1 or 2; Cs (95) = UCL95 concentration (mg/kg); Cs (max) = maximum concentration (mg/kg of soil); AUF = Area use factor, calculated as the site area/species home range (value cannot exceed 1.0); PS = fraction of soil ingestion as proportion of diet; FIR = Species-specific Food Ingestion Rate (kg food/kg body weight /d); NOAEL = No Observed Adverse Effect Level; NA = TRV not available

**Table 23**  
**Calculated and Reported Exposure Dose and EHQ**

Receptor	CAS Number	Chemical Name	0- to 2-ft Soil Sample Concentration							
			Exposure Dose ( $C_{95}$ ) (mg/kg/d)		EHQ ( $C_{95}$ )		Exposure Dose ( $C_{max}$ ) (mg/kg/d)		EHQ ( $C_{max}$ )	
			Calculated	Reported	Calculated	Reported	Calculated	Reported	Calculated	Reported
Western Meadowlark	121-14-2	2,4-Dinitrotoluene	1.41E-03	1.20E-03	NA	NA	1.11E-02	9.46E-03	NA	NA
Western Meadowlark	606-20-2	2,6-Dinitrotoluene	NA	NA	NA	NA	NA	NA	NA	NA
Western Meadowlark	2691-41-0	HMX	7.48E-02	6.37E-02	NA	NA	5.49E-01	4.66E-01	NA	NA
Western Meadowlark	99-35-4	1,3,5-Trinitrobenzene	9.36E-03	7.96E-03	NA	NA	2.19E-01	1.86E-01	NA	NA
Western Meadowlark	118-96-7	TNT	3.68E-02	3.13E-02	NA	NA	1.12E+00	9.51E-01	NA	NA
Swift Fox	121-14-2	2,4-Dinitrotoluene	1.01E-06	8.34E-07	4.12E-07	3.40E-07	7.91E-06	6.57E-06	3.23E-06	2.68E-06
Swift Fox	606-20-2	2,6-Dinitrotoluene	NA	NA	NA	NA	NA	NA	NA	NA
Swift Fox	2691-41-0	HMX	9.49E-06	7.90E-06	9.30E-06	7.75E-06	6.96E-05	5.77E-05	6.82E-05	5.66E-05
Swift Fox	99-35-4	1,3,5-Trinitrobenzene	2.51E-06	2.08E-06	1.06E-05	8.81E-06	5.89E-05	4.88E-05	2.50E-04	2.07E-04
Swift Fox	118-96-7	TNT	3.54E-05	2.94E-05	1.26E-04	1.04E-04	1.08E-03	8.93E-04	3.83E-03	3.17E-03
Ferruginous Hawk	121-14-2	2,4-Dinitrotoluene	1.34E-07	1.08E-07	NA	NA	1.05E-06	8.51E-07	NA	NA
Ferruginous Hawk	606-20-2	2,6-Dinitrotoluene	NA	NA	NA	NA	NA	NA	NA	NA
Ferruginous Hawk	2691-41-0	HMX	1.26E-06	1.02E-06	NA	NA	9.24E-06	7.48E-06	NA	NA
Ferruginous Hawk	99-35-4	1,3,5-Trinitrobenzene	3.33E-07	2.70E-07	NA	NA	7.81E-06	6.33E-06	NA	NA
Ferruginous Hawk	118-96-7	TNT	4.70E-06	3.81E-06	NA	NA	1.43E-04	1.16E-04	NA	NA
Deer Mouse	121-14-2	2,4-Dinitrotoluene	5.32E-02	5.31E-02	6.75E-03	6.70E-03	4.18E-01	4.18E-01	5.30E-02	5.30E-02
Deer Mouse	606-20-2	2,6-Dinitrotoluene	NA	NA	NA	NA	NA	NA	NA	NA
Deer Mouse	2691-41-0	HMX	2.78E+00	2.78E+00	8.48E-01	8.50E-01	2.04E+01	2.03E+01	6.22E+00	6.19E+00
Deer Mouse	99-35-4	1,3,5-Trinitrobenzene	3.49E-01	3.48E-01	4.59E-01	4.60E-01	8.17E+00	8.16E+00	1.08E+01	1.07E+01
Deer Mouse	118-96-7	TNT	1.39E+00	1.39E+00	1.53E+00	1.50E+00	4.24E+01	4.23E+01	4.67E+01	4.66E+01

(Continued)

Note: NA = NOAEL or data were not available.

Red Color = EHQ &gt; 1

For western meadowlark, area of 1.7 acres was used to calculate AUF, but TWEM accepts only integer values for area, so a value of 2 acres was input.

**Table 23 (Concluded)**

Receptor	CAS Number	Chemical Name	0- to 12.5-ft Soil Sample Concentration								
			Exposure Dose ( $C_{95}$ ) (mg/kg/d)		EHQ ( $C_{95}$ )		Exposure Dose ( $C_{max}$ ) (mg/kg/d)		EHQ ( $C_{max}$ )		
			Calculated	Reported	Calculated	Reported	Calculated	Reported	Calculated	Reported	
Western Meadowlark	121-14-2	2,4-Dinitrotoluene	3.89E-03	3.30E-03	NA	NA	1.96E-01	1.66E-01	NA	NA	
Western Meadowlark	606-20-2	2,6-Dinitrotoluene	2.52E-03	2.13E-03	NA	NA	7.86E-02	6.68E-02	NA	NA	
Western Meadowlark	2691-41-0	HMX	9.08E-02	7.70E-02	NA	NA	2.74E+00	2.33E+00	NA	NA	
Western Meadowlark	99-35-4	1,3,5-Trinitrobenzene	2.64E-01	2.24E-01	NA	NA	2.83E+00	2.41E+00	NA	NA	
Western Meadowlark	118-96-7	TNT	3.13E-02	2.67E-02	NA	NA	2.43E+00	2.07E+00	NA	NA	
Swift Fox	121-14-2	2,4-Dinitrotoluene	2.77E-06	2.29E-06	1.13E-06	9.35E-07	1.39E-04	1.16E-04	5.67E-05	4.73E-05	
Swift Fox	606-20-2	2,6-Dinitrotoluene	1.32E-06	1.09E-06	5.39E-07	4.45E-07	4.11E-05	3.41E-05	1.68E-05	1.39E-05	
Swift Fox	2691-41-0	HMX	1.15E-05	9.54E-06	1.13E-05	9.35E-06	3.48E-04	2.89E-04	3.41E-04	2.83E-04	
Swift Fox	99-35-4	1,3,5-Trinitrobenzene	7.09E-05	5.87E-05	3.00E-04	2.49E-04	7.59E-04	6.30E-04	3.22E-03	2.67E-03	
Swift Fox	118-96-7	TNT	3.01E-05	2.50E-05	1.07E-04	8.87E-05	2.34E-03	1.94E-03	8.30E-03	6.88E-03	
Ferruginous Hawk	121-14-2	2,4-Dinitrotoluene	3.67E-07	2.97E-07	NA	NA	1.85E-05	1.50E-05	NA	NA	
Ferruginous Hawk	606-20-2	2,6-Dinitrotoluene	1.75E-07	1.41E-07	NA	NA	5.45E-06	4.42E-06	NA	NA	
Ferruginous Hawk	2691-41-0	HMX	1.53E-06	1.24E-06	NA	NA	4.62E-05	3.74E-05	NA	NA	
Ferruginous Hawk	99-35-4	1,3,5-Trinitrobenzene	9.41E-06	7.61E-06	NA	NA	1.01E-04	8.16E-05	NA	NA	
Ferruginous Hawk	118-96-7	TNT	4.00E-06	3.24E-06	NA	NA	3.11E-04	2.52E-04	NA	NA	
Deer Mouse	121-14-2	2,4-Dinitrotoluene	1.46E-01	1.46E-01	1.85E-02	1.85E-02	7.36E+00	7.36E+00	9.34E-01	9.34E-01	
Deer Mouse	606-20-2	2,6-Dinitrotoluene	9.40E-02	9.39E-02	1.19E-02	1.19E-02	2.94E+00	2.94E+00	3.73E-01	3.73E-01	
Deer Mouse	2691-41-0	HMX	3.37E+00	3.36E+00	1.03E+00	1.02E+00	1.02E+02	1.02E+02	3.11E+01	3.11E+01	
Deer Mouse	99-35-4	1,3,5-Trinitrobenzene	9.83E+00	9.81E+00	1.29E+01	1.29E+01	1.05E+02	1.05E+02	1.38E+02	1.38E+02	
Deer Mouse	118-96-7	TNT	1.19E+00	1.19E+00	1.31E+00	1.31E+00	9.23E+01	9.21E+01	1.02E+02	1.02E+02	

## **Analysis of terrestrial demonstration**

The application described in this chapter provides a demonstration of ARAMS for a terrestrial ERA. Five COCs and four assessment endpoint species were considered. Data for two different soil concentrations ( $C_{95}$  and  $C_{max}$ ) and two depth intervals (0 to 2 and 0 to 12.5 ft) were evaluated. The EHQs based on  $C_{max}$  for deer mouse were greater than 1.0 at SWMU 17 for HMX, 1,3,5-trinitrobenzene, and 2,4,6-TNT in the upper and lower soil depths. The EHQs based on  $C_{95}$  for deer mouse were greater than 1.0 at SWMU 17 for HMX, 1,3,5-trinitrobenzene, and 2,4,6-TNT in the lower soil depths; however, in the upper depth, EHQ was higher than 1.0 only for TNT. All other EHQs for which a TRV was available were less than 1.0. Ferruginous hawk and western meadowlark EHQs were not determined for 2,4-dinitrotoluene, 2,6-dinitrotoluene, HMX, and 1,3,5-trinitrobenzene due to a lack of available TRVs. The soil concentration for 2,6-dinitrotoluene in the upper depth of 0 to 2 ft was not available.

The calculated risk results are identical to those reported in the ERA report for the deer mouse since the same parameters were used, thus verifying the calculations in TWEM and WEAP. Differences in TWEM computed doses compared with those reported were due to TWEM input format limitations, which were corrected after this study.

# **6 Summary, Conclusions, and Recommendations**

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## **Summary and Conclusions**

Demonstration applications of ARAMS for ERAs are described in this report. The purposes of the study were to identify data gaps or other deficiencies in ARAMS for ecological assessments and to verify formulations and solutions to the extent possible. The two field sites, LAFB for aquatic and PCD for terrestrial contamination, were selected among 21 identified sites that have reports on ERAs. Several criteria were considered in the evaluation and selection of sites. These included the availability of a well developed ecological conceptual model, the quantitative examination of exposure pathways and hazard/risk, a description of the formulations that were used to estimate exposure and hazard/risks, the availability and quality of site data, the information required for fate and transport models if such models are appropriate, and some understanding of the original source of the contamination. The amount and type of data available for each site greatly influenced site selection.

The LAFB demonstration focuses on a sub-reach of the Back River (Southwestern Branch). This sub-reach is approximately 3,000 m long, 100 m wide, with an average water depth of 1.5 m. Detailed characterizations of the exposure pathways for benthic invertebrates, Atlantic croaker, belted kingfisher, and mink were available. Reported risk estimates were compared to risk estimates by various ARAMS components. PCB (Aroclor 1254), arsenic, and benzo(a)pyrene were the contaminants selected for the LAFB application.

ARAMS, using the Known BBF module, yielded risks identical to those reported. Computed benthic invertebrate tissue concentrations using BSAF and TBP were in close agreement with measured values. Computed organic chemical tissue concentrations for fish using the Gobas (1993) model were over-estimated compared with measured values, indicating a need to improve the parameterization for this model. When using measured diet concentrations, ARAMS modules yielded identical doses and risks compared with those reported in the RI report. The available BCF value used for arsenic appears to be too low when comparing measured and computed tissue concentrations. The measured tissue and diet concentrations for inorganics would improve the results, which ARAMS can accommodate.

The site selected for the terrestrial demonstration was the TNT Washout Facility and Discharge System (SWMU 17) located in PCD. The site is located within a short-grass prairie community and adjacent to an open water area. At PCD, risks to a primary consumer/omnivore (deer mouse), an upper-tropic level mammalian predator (swift fox), and two upper trophic level avian predators (ferruginous hawk and western meadowlark) were evaluated. The chemicals of potential concern utilized in this demonstration included TNT, 2,4-dinitrotoluene and 2,6-dinitrotoluene, HMX, and 1,3,5-TNB. Evaluations were performed using maximum and UCL95 concentrations for soil samples collected over two depth intervals, 0 to 2 and 0 to 12 ft.

The calculated risk results for PCD are identical to those reported in the ERA report when the same input parameters were used, thus verifying the calculations in TWEM. Differences in TWEM-computed doses compared with those reported were due to TWEM input format limitations, which were corrected after this study.

## Recommendations

These applications revealed several recommended improvements for ARAMS. ARAMS improvements are identified for two general parts, databases and modules. Regarding databases, the recommendations pertain to the need to reduce data gaps. On this note, it is important to understand that ARAMS links to databases that are maintained outside of the realm of ARAMS development and maintenance. Thus, any improvements and expansion of these databases would have to be borne by the people responsible for those databases. Additionally, reducing data gaps for databases requires a dedicated, long-term laboratory research effort.

The ERED database provides a variety of TRV values for several assessment endpoint body parts, e.g., whole body, blood, liver, etc. However, in numerous cases, the ERED NOAEL values differed from the Langley RI report by several orders of magnitude for a selected body part. The magnitude of the EHQ is determined primarily by the choice of TRV. The ERED needs to be expanded to include TRVs for additional species. Likewise, the BSAF database needs to be expanded to include additional contaminants and species.

More experience is needed in applying the Gobas (1993) model for bio-accumulation of organic chemicals in fish for cases where measured fish tissue data are available. This experience will help in determining optimal parameterization of the model for improved accuracy. Additionally, there is a need for improved methods for estimating inorganic chemical tissue concentrations for fish and other aquatic organisms, including concentrations in diets of assessment endpoint organisms. Improving/expanding data in ERED and BSAF and developing improved methods for estimating tissue concentrations will require a strong laboratory research commitment that extends far beyond ARAMS developments.

There is a need for additional methods in ARAMS to estimate tissue concentrations in fish and in diets. Other than the stand-alone TrophicTrace model, TBP is the only other method presently available, and TBP is more appropriate for benthic organisms exposed to organic chemicals. At least two other modules have been identified as needed components that can be linked in ARAMS/FRAMES to other modules. One module is a BCF calculator where a specified BCF is multiplied by the water concentration to obtain tissue concentration. BCF values could be retrieved from a database, such as the Ecotox Database of USEPA. The other module is a dynamic Gobas model for fish, which exists in the FISHRAND model (Menzie-Cura & Associates, Inc. 2003). FISHRAND also allows modeling of multiple individuals of a population where each individual can migrate or is mobile over a spatial grid. At the time this report was prepared, work was under way to incorporate all three components (i.e., BCF module, FISHRAND, and Ecotox DCE for retrieving BCF values) into ARAMS.

The TrophicTrace model and documentation need improvements. For example, the user's manual and accompanying examples describe and display the use of 28-day bioassay results. However, the 28-day arsenic concentrations in the sandworm example do not appear to be utilized in any risk calculations (von Stackelberg and Burmistrova 2003). Also, the option "Reference Invertebrate" was not found in version 3.02. TrophicTrace food chain models need to be modified to allow user defined gastrointestinal absorption factors instead of using the same factor for all chemicals.

TrophicTrace TTF values existed only for arsenic, copper, lead, cadmium, and zinc. Additional TTF values are needed to more comprehensively estimate bioaccumulation from invertebrates to fish for hydrophilic organic and inorganic chemicals (von Stackelberg and Burmistrova 2003). von Stackelberg and Burmistrova (2003) list BCF values for only four chemicals, but additional BCF values are also needed. The Ecotox Database (<http://www.epa.gov/ecotox>) may help with this need. The arsenic BCF value in TrophicTrace may need to be revisited since TrophicTrace far underestimated arsenic tissue concentrations. In this application, TrophicTrace used the same BCF value to estimate benthic invertebrate, killifish, bivalves, and blue crab tissue concentrations of arsenic, which resulted in estimates that were inaccurate within two orders of magnitude. Local environmental conditions, such as Eh, pH, organic content, suspended solids, and temperature, can affect BCF, but models that account for these effects presently do not exist.

The ARAMS terrestrial modules could be improved by including more BAF data parameters within the BAF Database. This need was identified prior to this application and had been targeted to address. Also, TWEM input format restrictions were addressed as a result of this study.

# References

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- Arthur, W. J., and Alldredge, A. W. (1979). "Soil ingestion by mule deer in northcentral Colorado," *Journal of Range Management* 32(1), 67-71.
- Arthur, W. J., III, and Gates, R. J. (1988). "Trace element intake via soil ingestion in pronghorns and in black-tailed jackrabbits," *Journal of Range Management* 41(2), 162-166.
- Becthel Jacobs Company, LLC. (1998). "Biota sediment accumulation factors for invertebrates: Review and recommendations for the Oak Ridge Reservation," BJC/OR-112, prepared for the Office of Environmental Management, U.S. Department of Energy.
- Beyer, W. N., Conner, E. E., and Gerould, S. (1994). "Estimates of soil ingestion by wildlife," *J. Wildl. Mgmt.* 58(2), 375-382.
- Calder, W. A., III, and Braun, E. J. (1983). "Scaling of osmotic regulation in mammals and birds," *American Journal of Physiology* 244(13), R601-R606.
- Clarke, J. U., and McFarland, V. A. (1991). "Assessing bioaccumulation in aquatic organisms exposed to contaminated sediments," Miscellaneous Paper D-91-2, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.
- Cura, J. J., Heiger-Bernays, W., Bridges, T. S., and Moore, D. W. (1999). "Ecological and human health risk assessment guidance for aquatic environments," Technical Report DOER-4, U.S. Army Engineer Research and Development Center, Vicksburg, MS.
- Dillon, T. M., Suedel, B. C., Peddicord, R. K., Clifford, P. A., and Boraczek, J.A. (1995). "Trophic transfer and biomagnification potential of contaminants in aquatic ecosystems," *Environmental Effects of Dredging Technical Notes*, EEDP-01-33, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.
- Dixon, D. G., and Sprague, J. B. (1981). "Acclimation-induced changes in toxicity of arsenic and cyanide to rainbow trout, *Salmo gairdneri* Richardson," *J. Fish Biol.* 18, 579-589.

- Dunning, J. B., Jr. (1993). *CRC handbook of avian body masses*. CRC Press, Boca Raton.
- Earth Tech. (2002). "Sitewide screening ecological risk assessment Tiers 1 and 2 risk evaluation Pueblo Chemical Depot, Pueblo, Colorado, draft final," Contract Report, Englewood, CO.
- Gilbert, R. O. (1987). *Statistical methods for environmental pollution monitoring*. Van Nostrand Reinhold, New York.
- Gobas, F. A. P. C. 1993. "A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: Application to Lake Ontario," *Ecological Modelling* 69, 1-17.
- Hansen, D. J., Schimmel, S. C., and Forester, J. (1974). "Aroclor 1254 in eggs of sheepshead minnows: Effect on fertilization success and survival of embryos and fry." *Proceedings of Southeastern Game Fish Commission*.
- Hough J. L., Darrow, D., Eaton, J., and Baird, M. B. (1991). "Benzo(a)pyrene (BaP) treatment results in complete infertility in female pigeons," *Fed. Am. Soc. Exp. Biol.* 5, A882.
- Land, C. E. (1975). "Tables of confidence limits for linear functions for the normal mean and variance." *Selected tables in mathematical statistics, Vol III*. American Mathematical Society, Providence, RI, 385-419.
- Lanyon, W. E. (1994). "Western meadowlark (*Sturnella neglecta*).". A. Poole and F. Gill, ed., *The birds of North America*. No. 104, The Academy of Natural Sciences, Philadelphia and the American Ornithologists Union, Washington, DC.
- Mayoh, K. R., and Zach, R. (1986). "Grit ingestion by nestling tree swallows and house wrens," *Canadian Journal of Zoology* 64, 2090-2093.
- McCarty, L. S., and Mackay, D. (1993). "Enhancing ecotoxicological modeling and assessment: Body residues and modes of toxic action," *Environmental Science and Technology* 27, 1719-28.
- McCarty, L. S., Mackay D., Smith, A. D., Ozburn, G. W., and Dixon, D. G. (1992). "Residue-based interpretation of toxicity and bioconcentration QSARs from aquatic bioassays: Neutral narcotic organics," *Environmental Toxicology and Chemistry* 11, 917-30.
- McFarland, V. F. (1984). "Activity-based evaluation of potential bioaccumulation from sediments." *Proceedings of the Conference Dredging '84: Dredging and dredging material disposal*. Clearwater Beach, FL, 14-16 November 1984. R. L. Montgomery and J. W. Leach, ed., American Society of Civil Engineers, New York, 1, 461-467.

McFarland, V. F., and Clarke, J. U. (1986). "Testing availability of poly-chlorinated biphenyls from sediments using a two-level approach," USACE Committee on Water Quality, 6<sup>th</sup> Seminar: Proceedings. R. G. Willey, ed., Hydrologic Engineering Research Center, Davis, CA, 220-229.

McFarland, V. F., and Ferguson, P. W. (1995). "TBP revisited: A ten year perspective on a screening test for dredged sediment bioaccumulation potential." *Dredging '94: Proceedings of the Second International Conference on Dredging and Dredged Material Placement, Volume 1*. E. C. McNair, Jr., ed., sponsored by the Waterways Committee of the Waterway, Port, Coastal, and Ocean Division of the American Society of Civil Engineers.

Menzie-Cura & Associates, Inc. (2003). "FISHRAND, Probabilistic fish bio-accumulation model, user's manual, version 1.0," prepared for the Environmental Laboratory of the U.S. Army Engineer Research and Development Center by Menzie-Cura & Associates, Inc., Chelmsford, MA.

Nagy, K. A. (1987). "Field metabolic rate and food requirement scaling in mammals and birds," *Ecological Monographs* 57(2), 111-128.

Opresko, D. M., Suter, B. E., II, and Sample, G. W. (1996). "Toxicological benchmarks for wildlife: 1996 revision," DOE/ES/ER/TM-86/R3, Oak Ridge National Laboratory, Oak Ridge, TN.

Parsons Engineering Science, Inc. (1999). "Pueblo Chemical Depot Phase III RCRA facility investigation SWMU 17 final report," Contract Report, Denver, CO.

Pierce, A. M. (1974). "Energetics and water economy in the western meadowlark, *Sturnella neglecta*," *Diss. Abs. Int. (B)*, 35(11), 5723.

Radian International LLC. (1999). "Toxicity study – Langley Air Force Base," Austin, TX.

Ruiz, C. C., and Gerald, T. (2001). "RECOVERY Version 2.0, A mathematical model to predict the temporal response of surface water to contaminated sediments," Technical Report ERDC/EL TR-01-3, U.S. Army Engineer Research and Development Center, Vicksburg, MS.

Sample, B. E., Aplin, M. S., Efroymson, R. A., Suter, G. W., II, and Welsh, C. J. E. (1997). "Methods and tools for estimation of the exposure of terrestrial wildlife to contaminants," ORNL/TM-13391, Office of Environmental Policy and Assistance, U.S. Department of Energy, Oak Ridge National Laboratory, Oak Ridge, TN.

Schaeff, C., and Picman, J. (1988). "Destruction of eggs by western meadow-larks," *Condor* 90, 935-937.

- URS Corporation. (2002a). "Final remedial investigation report for ERP Site SS-63 Langley Air Force Base, Virginia, Volume 1," Contract Report, USAF Contract No. MUHJ-99-7114.
- \_\_\_\_\_. (2002b). "Final remedial investigation report for ERP Site SS-63 Langley Air Force Base, Virginia, Volume 2," Contract Report, USAF Contract No. MUHJ-99-7114.
- USACHPPM. (2004). "Development of terrestrial exposure and bioaccumulation information for the Army Risk Assessment Modeling System (ARAMS)," U.S. Army Center for Health Promotion and Preventive Medicine, Contract Number DAAD050-00-P-8365, Aberdeen Proving Ground, MD.
- U.S. Environmental Protection Agency. (1989). "Risk assessment guidance for Superfund, Volume 1 – Human health evaluation manual, Part A, Interim Final," EPA/540/1-89/0002, Publication 9285.701A, Office of Emergency and Remedial Response, Washington, DC.
- \_\_\_\_\_. (1992). "Supplement guidance to RAGS: Calculating the concentration term," Publication 92857-081, Office of Solid Waste and Emergency Response, Washington, DC.
- \_\_\_\_\_. (1993). "Wildlife exposure factors handbook, Volumes I and II," EPA/600/R-93/187, Office of Health and Environmental Assessment and Office of Research and Development, Washington, DC.
- \_\_\_\_\_. (1997). "Integrated Risk Information System (IRIS)," on-line computer database search.
- \_\_\_\_\_. (1997a). "Exposure factors handbook, Volume I: General factors," EPA/600/P-95/002Fa, Office of Research and Development, Washington, DC.
- \_\_\_\_\_. (1997b). Exposure factors handbook, Volume II: Food ingestion factors," EPA/600/P-95/002Fb, Office of Research and Development, Washington, DC.
- \_\_\_\_\_. (1999). "Data collection for the hazardous waste identification rule: Section 11.0, Aquatic food web data," prepared by the Center for Environmental Analysis for the Office of Solid Waste.
- U.S. Environmental Protection Agency/U.S. Army Corps of Engineers. (1998). "Evaluation of dredged material proposed discharge in waters of the U.S. testing manual: Inland testing manual," EPA 823-B-98-004.
- Virginia Water Quality Criteria (VWQC) for Surface Water. (1995). "Chronic Criteria for Protection of Aquatic Life."

von Stackelberg, K., and Bridges, T. S. (2002). "A management guide for a tiered risk assessment procedure for evaluating bioaccumulation data collected during regulatory evaluations of dredged material," Menzie-Cura & Associates, Inc., Chelmsford, MA, and U.S. Army Engineer Research and Development Center, Vicksburg, MS.  
<http://el.erdc.usace.army.mil/trophictrace/mgmtguide.pdf>

von Stackelberg, K., and Burmistrova, A. (2003). "TrophicTrace users manual: A tool for assessing risks from the trophic transfer of sediment-associated contaminants," Menzie-Cura & Associates, Chelmsford, MA.  
<http://el.erdc.usace.army.mil/trophictrace/ttmanual.pdf>

von Stackelberg, K., Vorhees, D., Linkov, I., Burmistrov, D., and Bridges, T. (2002). "Importance of uncertainty and variability to predicted risks from trophic transfer of contaminants in dredged sediments," *Risk Analysis* 22(3), 499-512.

Whelan, G., Castleton, K. J., Buck, J. W., Gelston, G. M., Hoopes, B. L., Pelton, M. A., Strenge, D. L., and Kickert, R. N. (1997). "Concepts of a Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES)," PNNL-11748, Pacific Northwest National Laboratory, Richland, WA.

Whelan, G., Pelton, M. A., Taira, R. Y., Rutz, F., and Gelston, G. M. (2000). "Demonstration of the wildlife ecological assessment program (WEAP)," PNNL-13395, Pacific Northwest National Laboratory, Richland, WA.

Wickwire, W. T., Menzie, C. A., Burmistrov, D., and Hope, B. K. (2004). "Incorporating spatial data into ecological risk assessments: The Spatially Explicit Exposure Module (SEEM) for ARAMS." *Landscape ecology and wildlife habitat evaluation: Critical information for ecological risk assessment, land use management activities, and biodiversity enhancement practices*, ASTM STP 1458, L. A. Kapustka, H. Galbraith, M. Luxon, and G. R. Biddinger, ed., ASTM International, West Conshohocken, PA.

Wirtz, J. R., and Fairbrother, A. (2001). "ARAMS terrestrial toxicity database background and description," prepared for USACHPPM by Parametrix, Corvallis, OR.

# **Appendix A**

## **List of Abbreviations and Acronyms**

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ARAMS	Adaptive Risk Assessment Modeling System
BAF	bioaccumulation factor
BBF	body burden concentration file
BCF	bioconcentration factor
BERA	baseline ecological risk assessment
BSAF	biota/sediment accumulation factor
CAS	Chemical Abstracts Service
CBR	critical body residue
CCC	criterion continuous concentration
COC	contaminant of concern
COPC	constituent of potential concern
COPEC	chemical of potential ecological concern
CSM	conceptual site model
DCE	data-client editor
DOE	U.S. Department of Energy
ED	effects dose, effective dose, exposure dose
EHQ	ecological hazard quotient
ERA	ecological risk assessment
ERDC	U.S. Army Engineer Research and Development Center
ERED	Environmental Residual-Effects Database
FDA	Food and Drug Administration
FRAMES	Framework for Risk Analysis in Multimedia Environmental Systems
FRANCO	FREQUENCY ANALYSIS OF CONCENTRATION
FS	Feasibility Study
FUDS	Formerly Used Defense Sites
GI	gastrointestinal absorption factor
GID	global input data
HHRA	human health risk assessment
HQ	hazard quotient
LAFB	Langley Air Force Base
LC	lethal concentration
LOAEL	lowest observed adverse effect level
LOED	lowest observable effects dose
MCPP	2-(2-methyl-4-chlorophenoxy) propionic acid

MRC	military relevant compound
MUI	module user interface
NASA	National Aeronautics and Space Administration
NOAEL	no observable adverse effect level
NOED	no observable effects dose
NOEL	no observable effects level
PAH	polycyclic aromatic hydrocarbons
PCB	polychlorinated biphenyls
PCD	Pueblo Chemical Depot
PCT	polychlorinated terphenyls
PNNL	Pacific Northwest National Laboratory
PRE	preliminary risk evaluation
RAGS	Risk Assessment Guidelines for Superfund
RBSL	risk based screening level
RI	Remedial Investigation
SEEM	Spatially Explicit Exposure Model
SERA	screening-level ecological risk assessment
SSL	soil screening level
SWMU	Solid Waste Management Unit
TBP	theoretical bioaccumulation potential
TNB	trinitrobenzene
TNT	trinitrotoluene
TOC	total organic carbon
TQ	toxicity quotient
TRV	toxicity reference value
TTD	Terrestrial Toxicity Database
TTF	trophic transfer factor
TWEM	Terrestrial Wildlife Exposure Model
TWI	terrestrial wildlife intake
USEPA	U.S. Environmental Protection Agency
WCF	water concentration file
WEAP	Wildlife Ecological Assessment Program

# **Appendix B**

## **TrophicTrace Output Using Calculated Concentrations as Input<sup>1</sup>**

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<sup>1</sup> All abbreviations and acronyms cited in this appendix can be found in the TrophicTrace Users Manual (von Stackelberg and Burmistrova 2003) located online at <http://el.erdc.usace.army.mil/trophictrace/ttmanual.pdf>



<b>Ecological Risk</b>									
<b>Summary for Mammals:</b>									
Mammal				Chemical of Concern				NOAEL Toxicity Quotient	LOAEL Toxicity Quotient
Mink: Organic				Aroclor 1254: Organic				6.76E-00	6.76E-01
								7.08E-00	7.08E-01
								7.77E-00	7.77E-01
								7.88E-00	7.88E-01
				Arsenic: Metal				2.28E-02	2.28E-03
								2.28E-02	2.28E-03
								2.28E-02	2.28E-03
				Benzo(a) pyrene: Organic				6.02E-00	6.02E-01
								6.29E-00	6.29E-01
								6.89E-00	6.89E-01
								6.97E-00	6.97E-01
<b>Summary for Avian:</b>									
Bird				Chemical of Concern				NOAEL TQ	LOAEL TQ
Belted Kingfisher: Organic				Aroclor 1254: Organic				8.74E-00	-
								9.43E-00	-
								1.09E+01	-

## **Summary for Fish:**

## Parameters

## **Chemical Parameters for Mammals:**

## Avian Parameters:

											2.29E+01
<b>Chemical Parameters for Birds:</b>											
Chemical of Concern			CAS	Bird		Average Daily Dose, mg/kg-day	NOAEL TRV, mg/kg-day	LOAEL TRV, mg/kg-day	BAF	NOAEL TRV for Eggs, mg/kg	LOAEL TRV for Eggs, mg/kg
Aroclor 1254: Organic			11097-69-1	Belted Kingfisher: Organic		3.85E-00	4.40E-01				
						4.15E-00	4.40E-01				
						4.81E-00	4.40E-01				
						4.90E-00	4.40E-01				
Arsenic: Metal			7440-38-2	Belted Kingfisher: Organic		1.12E-02	5.14E-00				
						1.12E-02	5.14E-00				
						1.12E-02	5.14E-00				
Benzo(a)pyrene: Organic			50-32-8	Belted Kingfisher: Organic		2.39E+01	8.47E-02				
						2.58E+01	8.47E-02				
						2.98E+01	8.47E-02				
						3.04E+01	8.47E-02				
<b>Chemical Parameters for Fish:</b>											
Chemical of Concern			CAS Number	Fish		NOAEL-Based CBR, mg/kg	LOAEL-Based CBR, mg/kg	BAF	NOAEL TRV for Eggs, mg/kg Lipid	LOAEL TRV for Eggs, mg/kg Lipid	
Aroclor 1254: Organic			11097-69-1	Atlantic Croaker: Organic		1.90E-00					

							1.90E-00				
							1.90E-00				
							1.90E-00				
Arsenic: Metal		7440-38-2	Atlantic Croaker: Organic				4.70E-01				
							4.70E-01				
							4.70E-01				
							4.70E-01				
Benzo(a) pyrene: Organic		50-32-8	Atlantic Croaker: Organic				1.90E-00				
							1.90E-00				
							1.90E-00				
							1.90E-00				
<b>Gobas Model Parameters</b>											
<b>Bioaccumulation in Fish:</b>											
Fish			Chemical of Concern		Use in Risk Assess- ment	Calculated Cf, ug/kg (wet weight)		Measured Cf, ug/kg (wet weight)		Conc. for Risk Assess- ment, ug/kg (wet weight)	
Atlantic Croaker: Organic			Aroclor 1254: Organic		Calculated	7.70E+03				7.70E+03	
						8.64E+03				8.64E+03	
						1.11E+04				1.11E+04	
						1.16E+04				1.16E+04	

			Benzo(a) pyrene: Organic		Calculated	4.87E+04				4.87E+04	
						5.47E+04				5.47E+04	
						6.97E+04				6.97E+04	
						7.27E+04				7.27E+04	
Killifish: Organic			Aroclor 1254: Organic		Calculated	4.64E+03				4.64E+03	
						5.05E+03				5.05E+03	
						5.93E+03				5.93E+03	
						6.06E+03				6.06E+03	
			Benzo(a) pyrene: Organic		Calculated	2.87E+04				2.87E+04	
						3.12E+04				3.12E+04	
						3.66E+04				3.66E+04	
						3.74E+04				3.74E+04	
<b>Fish Parameters:</b>											
Fish			Site		Trophic Level	Lipid Percent		Weight, g		Site Use Factor	
Atlantic Croaker			Organic		Piscivorous	5.42		230		1	
						5.42		230		1	
						5.42		230		1	
						5.42		230		1	
Killifish			Organic		Forage	2.65		3		1	
						2.65		3		1	
						2.65		3		1	
						2.65		3		1	



											5.93E+03
											6.06E+03
											2.87E+04
											3.12E+04
											3.66E+04
											3.74E+04
Killifish			Organic		Benthic Invertebrate: Organic		100	Aroclor 1254: Organic			3.96E+03
											3.96E+03
											3.96E+03
											3.96E+03
								Benzo(a) pyrene: Organic			2.60E+04
											2.60E+04
											2.60E+04

**Bioaccumulation Rates in Fish:**

Fish			Chemical		Qw	QI	K1	K2	Kd	Ke	Kg
Atlantic Croaker: Organic			Aroclor 1254: Organic		3.66E+01	3.66E-01	1.59E+02	2.67E-03	5.40E-02	1.08E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	2.67E-03	5.88E-02	1.18E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	2.67E-03	6.67E-02	1.33E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	2.67E-03	6.67E-02	1.33E-02	1.34E-02
			Benzo(a) pyrene: Organic		3.66E+01	3.66E-01	1.59E+02	3.14E-03	5.42E-02	1.08E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	3.14E-03	5.90E-02	1.18E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	3.14E-03	6.69E-02	1.34E-02	1.34E-02

					3.66E+01	3.66E-01	1.59E+02	3.14E-03	6.69E-02	1.34E-02	1.34E-02
Killifish: Organic		Aroclor 1254: Organic		2.71E-00	2.71E-02	9.02E+02	3.09E-02	1.04E-01	2.07E-02	3.20E-02	
				2.71E-00	2.71E-02	9.02E+02	3.09E-02	1.13E-01	2.25E-02	3.20E-02	
				2.71E-00	2.71E-02	9.02E+02	3.09E-02	1.28E-01	2.56E-02	3.20E-02	
				2.71E-00	2.71E-02	9.02E+02	3.09E-02	1.28E-01	2.56E-02	3.20E-02	
		Benzo(a) pyrene: Organic		2.71E-00	2.71E-02	9.02E+02	3.65E-02	1.04E-01	2.08E-02	3.20E-02	
				2.71E-00	2.71E-02	9.02E+02	3.65E-02	1.13E-01	2.26E-02	3.20E-02	
				2.71E-00	2.71E-02	9.02E+02	3.65E-02	1.28E-01	2.57E-02	3.20E-02	
				2.71E-00	2.71E-02	9.02E+02	3.65E-02	1.28E-01	2.57E-02	3.20E-02	
<b>Bioaccumulation in Invertebrates:</b>											
Inverte- brate			Diet Pathway	Lipid Percent	Chemical of Concern		Use in Risk Assess- ment	Calc. Conc., ug/kg (wet weight)	Measur. Conc., ug/kg (wet weight)	Conc. for Risk Assessmen t, ug/kg (wet weight)	
Bivalves: Organic			Sediment	1.06	Aroclor 1254: Organic		Calculated	3.96E+03		3.96E+03	
								3.96E+03		3.96E+03	
				1.06				3.96E+03		3.96E+03	
								3.96E+03		3.96E+03	
				1.06	Benzo(a) pyrene: Organic		Calculated	2.60E+04		2.60E+04	
								2.60E+04		2.60E+04	
				1.06				2.60E+04		2.60E+04	
								2.60E+04		2.60E+04	
Benthic Invertebrate: Organic			Sediment	1.06	Aroclor 1254: Organic		Calculated	3.96E+03		3.96E+03	
								3.96E+03		3.96E+03	
				1.06				3.96E+03		3.96E+03	

## **Chemicals Parameters:**

<b>BCF Approach Parameters</b>										
<b>Bioconcentration in Aquatic Species:</b>										
Species			Chemical of Concern		Use in Risk Assessment	Calculated Cf, ug/kg (wet weight)		Measured Cf, ug/kg (wet weight)		Conc. for Risk Assessment, ug/kg (wet weight)
Atlantic Croaker: Organic			Arsenic: Metal		Calculated	1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01
Killifish: Organic			Arsenic: Metal		Calculated	1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01
Bivalves: Organic			Arsenic: Metal		Calculated	1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01
Benthic Invertebrate: Organic			Arsenic: Metal		Calculated	1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01
Blue Crab: Organic			Arsenic: Metal		Calculated	1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01
						1.31E+01				1.31E+01

<b>Chemicals Parameters:</b>											
Chemical of Concern		Type	CAS	BCF	Log(Koc) or Kd	Cancer Slope Factor, 1/(mg/kg-day)	Ref. Dose, mg/kg-day	Sed. Conc., ng/g (dry weight)	Water Conc. Type	Water Conc., ng/L	Diss. Water Conc., ng/L
Arsenic		Metal	7440-38-2	3.5	3.9	1.5	3.00E-04	1.21E+04	Dissolved	3.74E+03	3.74E+03
				3.5	3.9	1.5	3.00E-04	1.21E+04		3.74E+03	3.74E+03
				3.5	3.9	1.5	3.00E-04	1.21E+04		3.74E+03	3.74E+03
				3.5	3.9	1.5	3.00E-04	1.21E+04		3.74E+03	3.74E+03

# **Appendix C**

## **TrophicTrace Output Using Measured Concentrations as Input<sup>1</sup>**

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<sup>1</sup> All abbreviations and acronyms cited in this appendix can be found in the TrophicTrace Users Manual (von Stackelberg and Burmistrova 2003) located online at <http://el.erdc.usace.army.mil/trophictrace/ttmanual.pdf>



<b><i>Ecological Risk</i></b>									
<b>Summary for Mammals:</b>									
Mammal				Chemical of Concern				NOAEL Toxicity Quotient	LOAEL Toxicity Quotient
Mink: Organic				Aroclor 1254: Organic				3.37E-00	3.37E-01
								3.37E-00	3.37E-01
								3.37E-00	3.37E-01
								3.37E-00	3.37E-01
				Arsenic: Metal				1.20E+01	1.20E-00
								1.20E+01	1.20E-00
								1.20E+01	1.20E-00
				Benzo(a) pyrene: Organic				3.01E-00	3.01E-01
								3.01E-00	3.01E-01
								3.01E-00	3.01E-01
								3.01E-00	3.01E-01
<b>Summary for Avian:</b>									
Bird				Chemical of Concern				NOAEL TQ	LOAEL TQ
Belted Kingfisher: Organic				Aroclor 1254: Organic				1.79E-01	—
								1.79E-01	—
								1.79E-01	—
				Arsenic: Metal				2.92E-01	—

								2.92E-01	–	–	–
								2.92E-01	–	–	–
								2.92E-01	–	–	–
				Benzo(a) pyrene: Organic				0.00E+01	–	–	–
								0.00E+01	–	–	–
								0.00E+01	–	–	–
								0.00E+01	–	–	–
								0.00E+01	–	–	–

**Summary for Fish:**

Fish				Chemical of Concern				NOAEL TQ	LOAEL TQ	NOAEL TQ for Eggs	LOAEL TQ for Eggs
Atlantic Croaker: Organic				Aroclor 1254: Organic				1.64E-02	–	–	–
								4.95E-02	–	–	–
								1.15E-01	–	–	–
								1.62E-01	–	–	–
				Arsenic: Metal				1.58E-00	–	–	–
								3.15E-00	–	–	–
								4.04E-00	–	–	–
								5.45E-00	–	–	–
				Benzo(a) pyrene: Organic				0.00E+01	–	–	–
								0.00E+01	–	–	–
								0.00E+01	–	–	–
								0.00E+01	–	–	–

## Parameters

## **Chemical Parameters for Mammals:**

## **Avian Parameters:**

											1.06E-01
							87				1.06E-01
								Arsenic: Metal			1.59E-00
											1.59E-00
		0.125	0.107	1			87				1.59E-00
											1.59E-00
								Benzo(a) pyrene: Organic			0.00E+01
							87				0.00E+01
											0.00E+01
											0.00E+01
		0.125	0.107	1	Blue Crab: Organic		13	Aroclor 1254: Organic			0.00E+01
											0.00E+01
											0.00E+01
							13				0.00E+01
								Arsenic: Metal			2.84E-00
											2.84E-00
		0.125	0.107	1			13				2.84E-00
											2.84E-00
								Benzo(a) pyrene: Organic			0.00E+01
							13				0.00E+01
											0.00E+01
											0.00E+01
<b>Chemical Parameters for Birds:</b>											
Chemical of Concern			CAS Number	Bird		Average Daily Dose, mg/kg-day	NOAEL TRV, mg/kg-day	LOAEL TRV, mg/kg-day	BAF	NOAEL TRV for Eggs, mg/kg	LOAEL TRV for Eggs, mg/kg

Aroclor 1254: Organic			11097-69-1	Belted Kingfisher: Organic		7.89E-02	4.40E-01				
						7.89E-02	4.40E-01				
						7.89E-02	4.40E-01				
						7.89E-02	4.40E-01				
Arsenic: Metal			7440-38-2	Belted Kingfisher: Organic		1.50E-00	5.14E-00				
						1.50E-00	5.14E-00				
						1.50E-00	5.14E-00				
						1.50E-00	5.14E-00				
Benzo(a) pyrene: Organic			50-32-8	Belted Kingfisher: Organic		0.00E+01	8.47E-02				
						0.00E+01	8.47E-02				
						0.00E+01	8.47E-02				
						0.00E+01	8.47E-02				

#### Chemical Parameters for Fish:

Chemical of Concern			CAS Number	Fish			NOAEL-Based CBR, mg/kg	LOAEL-Based CBR, mg/kg	BAF	NOAEL TRV for Eggs, mg/kg Lipid	LOAEL TRV for Eggs, mg/kg Lipid
Aroclor 1254: Organic			11097-69-1	Atlantic Croaker: Organic			1.90E-00				
							1.90E-00				
							1.90E-00				
							1.90E-00				
Arsenic: Metal			7440-38-2	Atlantic Croaker: Organic			4.70E-01				
							4.70E-01				
							4.70E-01				
							4.70E-01				

Benzo(a)pyrene: Organic			50-32-8	Atlantic Croaker: Organic			1.90E-00				
							1.90E-00				
							1.90E-00				
							1.90E-00				
<b>Gobas Model Parameters</b>											
<b>Bioaccumulation in Fish:</b>											
Fish			Chemical of Concern		Use in Risk Assessment	Calculated Cf, ug/kg (wet weight)		Measured Cf, ug/kg (wet weight)		Conc. for Risk Assessment, ug/kg (wet weight)	
Atlantic Croaker: Organic			Aroclor 1254: Organic		Measured	2.64E+03		3.11E+01		3.11E+01	
						2.88E+03		9.41E+01		9.41E+01	
						3.45E+03		2.19E+02		2.19E+02	
						3.57E+03		3.08E+02		3.08E+02	
			Benzo(a)pyrene: Organic		Measured	1.66E+04		0.00E+01		0.00E+01	
						1.80E+04		0.00E+01		0.00E+01	
						2.16E+04		0.00E+01		0.00E+01	
						2.23E+04		0.00E+01		0.00E+01	
Killifish: Organic			Aroclor 1254: Organic		Measured	4.90E+03		1.06E+02		1.06E+02	
						5.32E+03		1.06E+02		1.06E+02	
						6.25E+03		1.06E+02		1.06E+02	
						6.39E+03		1.06E+02		1.06E+02	

## Fish Parameters:

## Fish Diets:

											3.56E+01
											4.37E+01
											4.37E+01
											4.37E+01
											4.37E+01
					Benthic Invertebrate: Organic	33.3	Aroclor 1254: Organic				4.18E+03
											4.18E+03
											4.18E+03
											4.18E+03
							Benzo(a) pyrene: Organic				2.74E+04
											2.74E+04
											2.74E+04
											2.74E+04
					Killifish: Organic	33.4	Aroclor 1254: Organic				1.06E+02
											1.06E+02
											1.06E+02
							Benzo(a) pyrene: Organic				0.00E+01
											0.00E+01
											0.00E+01
Killifish			Organic		Benthic Invertebrate: Organic	100	Aroclor 1254: Organic				4.18E+03
											4.18E+03
											4.18E+03
							Benzo(a) pyrene: Organic				2.74E+04

											2.74E+04
											2.74E+04
											2.74E+04
<b>Bioaccumulation Rates in Fish:</b>											
Fish			Chemical		Qw	QI	K1	K2	Kd	Ke	Kg
Atlantic Croaker: Organic			Aroclor 1254: Organic		3.66E+01	3.66E-01	1.59E+02	2.67E-03	5.40E-02	1.08E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	2.67E-03	5.88E-02	1.18E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	2.67E-03	6.67E-02	1.33E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	2.67E-03	6.67E-02	1.33E-02	1.34E-02
			Benzo(a) pyrene: Organic		3.66E+01	3.66E-01	1.59E+02	3.14E-03	5.42E-02	1.08E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	3.14E-03	5.90E-02	1.18E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	3.14E-03	6.69E-02	1.34E-02	1.34E-02
					3.66E+01	3.66E-01	1.59E+02	3.14E-03	6.69E-02	1.34E-02	1.34E-02
Killifish: Organic			Aroclor 1254: Organic		2.71E-00	2.71E-02	9.02E+02	3.09E-02	1.04E-01	2.07E-02	3.20E-02
					2.71E-00	2.71E-02	9.02E+02	3.09E-02	1.13E-01	2.25E-02	3.20E-02
					2.71E-00	2.71E-02	9.02E+02	3.09E-02	1.28E-01	2.56E-02	3.20E-02
					2.71E-00	2.71E-02	9.02E+02	3.09E-02	1.28E-01	2.56E-02	3.20E-02
			Benzo(a) pyrene: Organic		2.71E-00	2.71E-02	9.02E+02	3.65E-02	1.04E-01	2.08E-02	3.20E-02
					2.71E-00	2.71E-02	9.02E+02	3.65E-02	1.13E-01	2.26E-02	3.20E-02
					2.71E-00	2.71E-02	9.02E+02	3.65E-02	1.28E-01	2.57E-02	3.20E-02
					2.71E-00	2.71E-02	9.02E+02	3.65E-02	1.28E-01	2.57E-02	3.20E-02

Bioaccumulation in Invertebrates:										
Invertebrate			Diet Pathway	Lipid Percent	Chemical of Concern		Use in Risk Assessment	Calc. Conc., ug/kg (wet weight)	Measur. Conc., ug/kg (wet weight)	Conc. for Risk Assessment, ug/kg (wet weight)
Bivalves: Organic			Sediment	1.06	Aroclor 1254: Organic		Measured	3.96E+03	3.56E+01	3.56E+01
								3.96E+03	3.56E+01	3.56E+01
				1.06				3.96E+03	3.56E+01	3.56E+01
								3.96E+03	3.56E+01	3.56E+01
				1.06	Benzo(a) pyrene: Organic		Measured	2.60E+04	4.37E+01	4.37E+01
								2.60E+04	4.37E+01	4.37E+01
								2.60E+04	4.37E+01	4.37E+01
				1.06				2.60E+04	4.37E+01	4.37E+01
								2.60E+04	4.37E+01	4.37E+01
Benthic Invertebrate: Organic			Sediment	1.06	Aroclor 1254: Organic		Measured	3.96E+03	4.18E+03	4.18E+03
								3.96E+03	4.18E+03	4.18E+03
				1.06				3.96E+03	4.18E+03	4.18E+03
								3.96E+03	4.18E+03	4.18E+03
				1.06	Benzo(a) pyrene: Organic		Measured	2.60E+04	2.74E+04	2.74E+04
								2.60E+04	2.74E+04	2.74E+04
								2.60E+04	2.74E+04	2.74E+04
				1.06				2.60E+04	2.74E+04	2.74E+04
								2.60E+04	2.74E+04	2.74E+04
Blue Crab: Organic			Sediment	0.933	Aroclor 1254: Organic		Measured	3.49E+03	0.00E+01	0.00E+01
								3.49E+03	0.00E+01	0.00E+01
				0.933				3.49E+03	0.00E+01	0.00E+01
								3.49E+03	0.00E+01	0.00E+01
				0.933	Benzo(a) pyrene:		Measured	2.29E+04	0.00E+01	0.00E+01

## **Chemicals Parameters:**

## BCF Approach Parameters

Bioconcentration in Aquatic Species:										
Species			Chemical of Concern		Use in Risk Assessment	Calculated Cf, ug/kg (wet weight)		Measured Cf, ug/kg (wet weight)		Conc. for Risk Assessment, ug/kg (wet weight)
Atlantic Croaker: Organic			Arsenic: Metal		Measured	1.31E+01		7.42E+02		7.42E+02
						1.31E+01		1.48E+03		1.48E+03
						1.31E+01		1.90E+03		1.90E+03

						1.31E+01		2.56E+03		2.56E+03	
Killifish: Organic			Arsenic: Metal		Measured	1.31E+01		1.59E+03		1.59E+03	
						1.31E+01		1.59E+03		1.59E+03	
						1.31E+01		1.59E+03		1.59E+03	
						1.31E+01		1.59E+03		1.59E+03	
Bivalves: Organic			Arsenic: Metal		Measured	1.31E+01		1.43E+03		1.43E+03	
						1.31E+01		1.43E+03		1.43E+03	
						1.31E+01		1.43E+03		1.43E+03	
						1.31E+01		1.43E+03		1.43E+03	
Benthic Invertebrate: Organic			Arsenic: Metal		Measured	1.31E+01		1.21E+04		1.21E+04	
						1.31E+01		1.21E+04		1.21E+04	
						1.31E+01		1.21E+04		1.21E+04	
						1.31E+01		1.21E+04		1.21E+04	
Blue Crab: Organic			Arsenic: Metal		Measured	1.31E+01		2.84E+03		2.84E+03	
						1.31E+01		2.84E+03		2.84E+03	
						1.31E+01		2.84E+03		2.84E+03	
						1.31E+01		2.84E+03		2.84E+03	

**Chemicals Parameters:**

Chemical of Concern		Type	CAS Number	BCF	Log(Koc) or Kd	Cancer Slope Factor, 1/(mg/kg- day)	Ref. Dose, mg/kg-day	Sed. Conc., ng/g (dry weight)	Water Conc. Type	Water Conc., ng/L	Diss. Water Conc., ng/L
Arsenic		Metal	7440-38-2	3.5	3.9	1.5	3.00E-04	1.21E+04	Dissolved	3.74E+03	3.74E+03
				3.5	3.9	1.5	3.00E-04	1.21E+04		3.74E+03	3.74E+03
				3.5	3.9	1.5	3.00E-04	1.21E+04		3.74E+03	3.74E+03
				3.5	3.9	1.5	3.00E-04	1.21E+04		3.74E+03	3.74E+03

# REPORT DOCUMENTATION PAGE

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<b>13. SUPPLEMENTARY NOTES</b>					
<b>14. ABSTRACT</b>  The Adaptive Risk Assessment Modeling System (ARAMS) has been developed for the Army to provide the capability to conduct risk assessments associated with exposure to constituents of potential concern. ARAMS provides a reliable and repeatable methodology for conducting collaborative and comparative risk assessments, thus providing a savings in time and cost for conducting such assessments and potentially leading to significant remediation cost savings by providing more accurate risk-based cleanup targets. The objectives of this study were to describe and demonstrate the application of ARAMS for ecological risk characterization at two field sites, an aquatic site and a terrestrial site. Other purposes of the study were to identify errors and data/development gaps, and to validate methods and solutions of ARAMS and its components for ecological risk assessment. ERDC researchers, through literature searches and communications with personnel at the Corps of Engineers Center of Expertise for Hazardous, Toxic, and Radiological Waste and Corps districts, identified potential demonstration sites. The candidate sites, which are or were owned or operated by the U.S. Army, Navy, or Air Force, were either components of Superfund projects or were Formerly Used Department of Defense Sites. Langley Air Force Base (LAFB) and Pueblo Chemical Depot (PCD) were selected among the identified sites to demonstrate the capabilities of ARAMS.					
(Continued)					
<b>15. SUBJECT TERMS</b> ARAMS Demonstration Terrestrial site Aquatic site Ecological risk					
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**14. (Concluded)**

The reported ecological risk assessments for LAFB and PCD sites were used to obtain data for conducting these demonstrations. At LAFB, risks were evaluated for benthic invertebrates, a fish (Atlantic croaker), a piscivorous bird (belted kingfisher), and a carnivorous mammal (mink). The selected chemicals of concern at LAFB were polychlorinated biphenyls, benzo(a)pyrene, and arsenic. At PCD, risks to a primary consumer/omnivore (deer mouse), an uppertropic level mammalian predator (swift fox), and two upper trophic level avian predators (ferruginous hawk and western meadowlark) were evaluated. The chemicals of concern at PCD were 2,4,6-trinitrotoluene, 2,4-dinitrotoluene, 2,6-dinitrotoluene, cyclotetramethylene-tetrinitramine, and 1,3,5-trinitrobenzene. These applications illustrate a number of ARAMS features, including media fate and transport, access to aquatic and terrestrial databases to extract wildlife toxicity benchmarks, and calculations of exposure doses and hazards quotients.